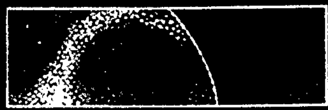
High Performance Computing

contributions to

DoD Mission Success 1998



CSM
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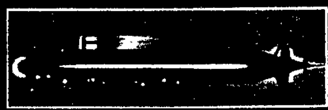

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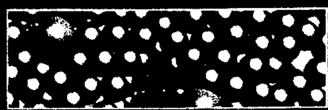

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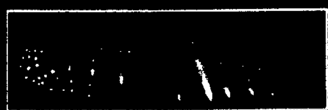

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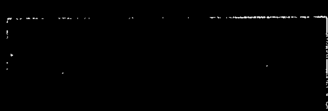

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High Performance Computing contributions to DoD Mission Success 1998

May 1998

OFFICE OF THE DIRECTOR OF
DEFENSE RESEARCH AND ENGINEERING

WASHINGTON, DC 20301-3040

Thanks to the continuing efforts of our team of government, contractor, HPC industry, and academic partners, the High Performance Computing Modernization Program has provided a powerful high-end HPC environment to the DoD science and technology and the developmental test and evaluation communities. The Program's real success, however, lies in the degree that our users leverage this capability to deliver technological advantage to the warfighter. It is this type of success that we are presenting in the 1998 edition of *High Performance Computing Contributions to DoD Mission Success*. Accordingly, the 100 success stories presented here highlight the scope and diversity of mission results that are being achieved using the HPC Modernization Program resources.

Cutting across all ten computational technology areas, from a scientific perspective, as well as the Joint Warfighting Capability Objectives defined by the Joint Chiefs of Staff, these success stories recognize outstanding accomplishments of DoD scientists and engineers. While many of the projects are focused on generic defense science challenges, this year's collection also foreshadows the growing importance of high performance computing in acquisition of the next generation of warfighter systems. Included, for example, are projects explicitly related to the Navy Seawolf submarine (p. 26), the Army M1 tank (p. 31), the Air Force F-22 (p. 42), Army/Air Force airborne parachute drops (p. 44), theater missile defense (p. 129), and anti-terrorism (p. 57). For these and similar major programs, high performance computing is on the critical path. New materials, better fuels, stealth characteristics, vulnerability, external stores, and the basic aerodynamic and structural design of the entire platform–all are represented in this volume, and all require high performance computing.

Beyond the mission impact of outstanding work that is represented, these results are indicative of the future requirements that will be fundamental to defense competitiveness in the 21st century. Ensuring that these capabilities will be available first to the DoD community will be a continuing high priority for years to come.

Tom Dunn

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Director
High Performance Computing
Modernization Program

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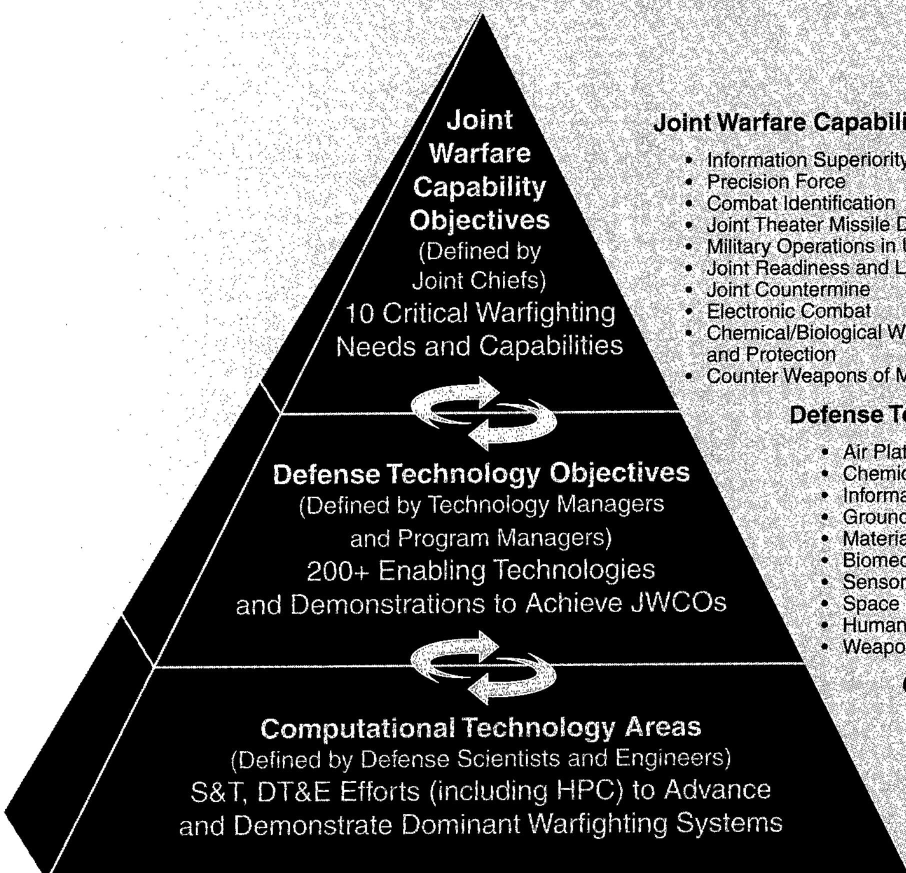


Joint Warfare Capability Objectives

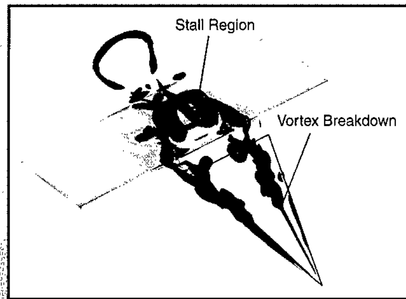
- Information Superiority
- Precision Force
- Combat Identification
- Joint Theater Missile Defense
- Military Operations in Urban Terrain
- Joint Readiness and Logistics
- Joint Countermine
- Electronic Combat
- Chemical/Biological Warfare Defense and Protection
- Counter Weapons of Mass Destruction

Defense Technology Objectives

- Air Platforms
- Chemical/Biological Defense and Nuclear
- Information Systems Technology
- Ground and Sea Vehicles
- Materials and Processes
- Biomedical
- Sensors, Electronics, and Battlespace Environment
- Space Platforms
- Human Systems
- Weapons

Computational Technology Areas

- Structural Mechanics
- Fluid Dynamics
- Chemistry and Materials
- Electromagnetics and Acoustics
- Weather and Ocean Modeling
- Signal-Image Processing
- Forces Modeling and Simulation
- Environmental Quality Modeling and Simulation
- Electronics and Nanoelectronics
- Integrated Modeling and Test Environments



JWCO
DTO
CTA

Example:

Capability Need (JWCO) - Joint Readiness and Logistics

"Gain decisive advantage by controlling the breadth, depth, and height of the battlespace, guarantee air superiority and sustainment at strategic, operational, and tactical levels of operation."

Enabling Technologies (DTO) - Air Platforms

"Validate advanced technologies in a realistic operational environment that demonstrate affordable aerodynamic technologies, improved performance and predict the effects of unsteady aerodynamics to increase fatigue life and reduce support costs."

HPC Computational Technology Area (CTA) - Computational

Modeling Control Surfaces of High Performance Aircraft - "extensive modeling and simulation of the aerodynamic flows that enhance the maneuverability and agility of high performance aircraft and measure the adverse impact upon the loss of control, structural fatigue and component failure. The significance is increased effectiveness and lethality of the weapon system, lower maintenance costs and increased readiness."

Joint Warfare Capability Objective

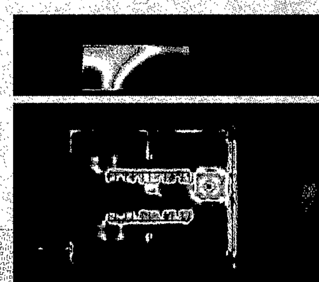
- Information Superiority

Defense Technology Objective

- Sensors, Electronics, and Battlespace Environment

Computational Technology Areas

- Signal-Image Processing
- Computational Fluid Dynamics



JWCO
DTO
CTA

Example:

Joint Warfare Capability Objective

- Chemical/Biological Warfare Defense and Protection

Defense Technology Objective

- Chemical/Biological Defense and Nuclear

Computational Technology Area

- Computational Fluid Dynamics

Capability Need (JWCO) - Chemical/Biological (CB) Warfare Defense and Protection

"Develop a simulation capability that integrates all available sensor data with other relevant data to provide commanders with a decision aid to determine appropriate protective posture and actions to avoid contamination."

Enabling Technologies (DTO) - Chemical/ Biological Defense

"Develop operational support systems that provide situational awareness and aid command evaluations, integrate sensor data, and predict realistic training and simulation of the chemical/biological battlefield environment."

HPC Computational Technology Area (CTA) - Computational Fluid Dynamics

Contaminant Transport Modeling for Consequence Management - "Significantly improving DoDs modeling and simulation capability to help counter the threat posed by the proliferation of chemical and biological weapons worldwide. The need is aimed at providing a timely, effective response to a chemical/biological threat or to assess the effects of an obscurant cloud."

The Enabling Technology for Putting the Best Capability in the Hands of the Customer — THE WARFIGHTER...

HPC Enables DoD Mission Success

HIGH PERFORMANCE COMPUTING IN DoD

High Performance Computing (HPC) is a key, enabling technology that is essential to assure that U.S. Forces maintain dominance on the battlefield with minimal risk to life, even against numerically superior forces. Tracing requirements from the President's National Security Strategy to our National Military Strategy as defined by the Military Services, Joint Chiefs of Staff, and the warfighting Commanders in Chief (CINCs), one common denominator prevails—the need for militarily superior technology. Technology is a key discriminator in our deterrence of conflicts; failing to deter aggression, technology can be the difference between success and failure on the battlefield.

HPC enables advanced modeling and simulation concepts and capabilities that can be used to assess the value of individual components or new weapon systems' projected performance levels. Data collected from modeling and simulation will assist milestone decisions by pointing to research, development, test and evaluation (RDT&E) of most value to the warfighter. Through the use of HPC resources for example, it is possible to simulate the capabilities of a new weapon system and to measure that system's impact on existing tactics and the predicted outcome of a military engagement (using tens of thousands of entity types). As a result, senior DoD leadership will have data to assist in the decision-making process as early as possible. These data will provide information about whether to proceed, modify, or cancel a program and where to best invest our RDT&E resources. Other mission-critical areas that could be greatly improved by advanced modeling and simulations using HPC include ocean modeling and weather prediction, bomb damage assessment, water tampering determinations, modeling of radio frequency systems and antenna designs, environmental impacts/cleanup, and counter-proliferation and counter-terrorism scenarios. Providing a "world-class" high performance computing environment ensures that DoD user applications can take full advantage of technological change.

Timely solutions to increasingly complex scientific and technology-related problems require the use of high performance computing and communications measured in trillions of floating-point operations per second (teraFLOPS). Examples of applications requiring these capabilities include computational fluid dynamics, improved radar cross section prediction and target recognition, development of new high-temperature structural materials, signal and image processing, and advanced weapons and defense systems based on electromagnetics and acoustics.

Modern, scalable, high performance parallel computing systems, including advanced software compilers, debuggers, and programming tools, are needed to support mission-specific and common-user applications and algorithms. Many key defense applications require massive, hierarchical data storage along with data visualization capabilities to provide meaningful results to key decision makers in a timely manner. Software capable of supporting high performance computing applications is also essential. Identifying and developing or acquiring

the software tools that function effectively in a shared HPC environment requires cooperation and teaming among government, industry, and academia to minimize costs and maintain standards. High-speed connectivity is required for sharing data and accessing high performance computer systems from remote locations and must be commensurate with the input/output (I/O) bandwidth requirements of each application and HPC system. Bandwidth requirements are projected to approach more than 600 million bits per second (bps). Thus, it is apparent that high performance computing, including the hardware, software, and communications, is one of the most powerful and unique enabling technologies for conducting critical research and engineering to develop and deploy technologically superior weapon systems and forces planning concepts. HPC will assist greatly in maintaining and advancing our technology edge on the battlefield that will reduce risk to life, minimize the costs of acquisitions, and maximize the use of each system operating in a joint warfighting environment.

THE DoD HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM (HPCMP)

History

The High Performance Computing Modernization Program (HPCMP) was initiated in FY 1993 in response to congressional direction to modernize the DoD HPC capabilities. Early on, senior leaders recognized the unique potential of this emerging technology as critical to our nation's future defense. The High Performance Computing Modernization Office (HPCMO), staffed with representatives from each Service, was established in FY 1994 to perform life cycle management and acquisition oversight needed to ensure that the program supports the HPC needs of the defense science and technology (S&T) and developmental test and evaluation (DT&E) communities. Since FY 1996, the program has fielded a world-class HPC infrastructure, available to the full S&T and DT&E communities, that includes 4 major shared resource centers (MSRCs) and 13 smaller focused distributed centers (DCs) across the country.

Program Scope

The HPCMP scope is bounded both in terms of the user community it serves and the technological capability it delivers. By limiting the scope and by concentrating the majority of resources at a small number of shared centers, the program has been able to provide world-class computing capabilities that could not have efficiently been obtained and sustained by individual Services or Agencies. This sharing of resources reduces overall acquisition and sustainment costs and fosters collaboration and cooperation across the DoD S&T and DT&E communities.

The HPCMP user community is defined by Congress (Public Law 104-61, December 1, 1995, 109 Statute 665, Sec. 8073) to be

> *"….. (1) the DoD Science and Technology (S&T) sites under the cognizance of the Director, Defense Research and Engineering, (2) the DoD Test and Evaluation (DT&E) centers under the Director, Test and Evaluation (Office of the Under Secretary of Defense, Acquisition and Technology), and (3) the Ballistic Missile Defense Organization . ."*

While the program serves the DT&E community, it is important to note that its scope does not currently address operational test and evaluation requirements — including live fire testing. Nor is it funded sufficiently to address many of the unique applications that are not easily handled at multiuser shared centers such as those maintained by this program. Recognizing these limitations, and in response to congressional reporting requirements,* the Director, Developmental Test, Systems Engineering and Evaluation, and the Director, Operational Test and Evaluation, are currently developing a separate plan for integrating HPC fully into the production test and evaluation process and enterprise.

**National Defense Authorization Act for Fiscal Year 1996*, Conference Report 104-450, pp 701-702.

From a technology capability perspective, the program maintains a strict focus on providing high performance computing. The definition of "high performance computing" changes as the technology continues to evolve. This consistent evolution requires that the program continually reassess its acquisition plans to ensure that it is not acquiring systems that have become "departmental" class — computational capability that remains the responsibility of the local mission organization. The rapid evolution of high performance computing also requires that the program focus on delivering improved capability early in its commercial life cycle. This allows the DoD to maintain the technological edge required to analyze, design, produce, and deploy advanced weapons systems and capabilities to the warfighter — before similar computational capabilities are available to our adversaries and economic competitors.

Shared Resource Centers

The HPCMP consists of three focused initiatives: the high performance computing shared resource centers (MSRCs and DCs), the Defense Research and Engineering Network (DREN), and the Common High Performance Computing Software Support Initiative (CHSSI).

Four Major Shared Resource Centers (MSRCs) were established with a full suite of HPC capabilities. The MSRC infrastructure includes completely networked HPC environments, leading-edge computational systems, scientific visualization tools, hierarchical storage capabilities, and a tailored HPC programming environment, including training and user support/computational area expertise. Table 1 identifies the HPC resources installed at the MSRCs.

Table 1 — Major Shared Resource Center HPC Capability (as of June 1998)

Location	DoD HPCMP System	Number of Processors	Total Memory (gigabytes)	Total Capability (Peak gigaflops)
Army Corps of Engineers Waterways Experiment Station	Cray C90	16	8	16
	IBM SP	256	256	138
	Cray T3E	336	86	302
	IBM SP P2SC	126	63	81
	SGI Origin 2000	128	64	51
Naval Oceanographic Office	Cray C90	16	8	16
	SGI Origin 2000	128	64	51
	Cray T90	24	8	58
	SGI PowerChallenge	52	16	19
	Cray J932SE (Classified)	12	4	2
	SGI PowerChallenge (Classified)	8	4	3
	Cray T3E	544	139	490
Army Research Laboratory	SGI Origin 2000	288	160	115
	Cray T90	12	8	22
	SGI Origin 2000 (Secret)	64	32	26
	Cray T90 (Secret)	8	4	14
	Cray J932SE (Special Access)	16	32	3
	Cray J932SE (Special Access)	16	8	3
	SGI Origin 2000 (Special Access)	32	12	13
Aeronautical Systems Center	Cray C90	16	8	16
	IBM SP	256	264	138
	SGI Origin 2000	512	320	205
	SGI PowerChallenge	16	8	6

Thirteen Distributed Centers (DCs) complement the MSRCs and provide site-unique HPC support. The DC high performance computing systems are typically in the small to medium size range, and several centers focus primarily on real-time applications requiring dedicated resources. As necessary, DCs supplement MSRC processing and evaluate new high performance computing hardware. Table 2 identifies the HPC resources installed by the HPCMP at each of the DCs. Note that, unlike the MSRCs, DCs may have additional HPC computers installed that are dedicated to local mission requirements.

Table 2 — Distributed Center HPCMP Resources (as of March 1998)

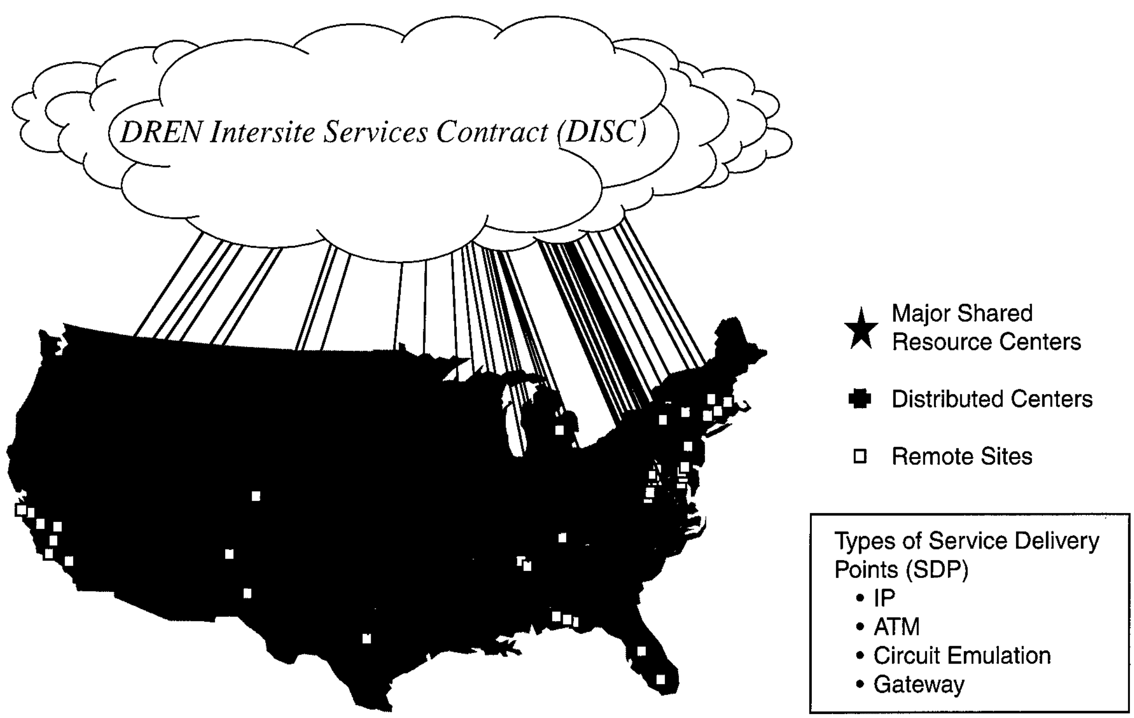
Location	DoD HPCMP System	Processors	Total Memory (gigabytes)	Total Capability (Peak gigaflops)
Air Force Arnold Engineering Development Center (AEDC)	Convex C4640 Convex C4640 (Classified) Convex Exemplar SPP-2000 HP Exemplar X (Classified) SGI Origin 2000	4 4 64 48 64	4 4 16 11 32	3 3 46 34 26
Air Force Development Test Center (AFDTC)	Cray T3D SGI Onyx	128 32	8 8	19 12
Air Force Maui High Performance Computing Center (MHPCC)	IBM SP (Classified) IBM SP IBM P2SC IBM SMP IMB P2SC	96 192 51 64 192	13 31 7 8 96	26 51 25 14 123
Air Force Research Laboratory (Rome)*	Intel Paragon	321	21	30
Army High Performance Computing Research Center (AHPCRC)	Cray T3E	272	139	326
Army Redstone Technical Test Center (RTTC)	SGI Origin 2000 SGI Origin 2000 (Classified)	32 32	7 7	13 13
Army Space and Missile Defense Command (SMDC)	SGI Origin 2000 SGI Origin 2000 SGI Origin 2000 SGI Origin 2000 SGI Origin 2000	64 32 32 32 128	16 10 10 10 32	26 13 13 13 52
Army Tank-Automotive RD&E Center (TARDEC)	SGI PowerChallenge	64	16	24
Army White Sands Missile Range (WSMR)*	TMC CM-500 SGI Origin 2000	128 64	16 24	20 26
Naval Air Warfare Center (NAWC)	SGI PCA (Classified) SGI Onyx2 (Classified) SGI Onyx2 (Classified)	40 32 32	12 16 8	15 13 13
Naval Research Laboratory (NRL)*	TMC CM-500e TMC CM-500e Convex Exemplar SPP-2000 SGI Origin 2000	256 32 64 128	33 4 16 32	41 5 46 52
Naval Undersea Warfare Center (NUWC)	Cray T3D	64	4	10
Naval SPAWAR System Center, San Diego (SSCSD)*	Intel Paragon (Classified) Convex Exemplar SPP-1000	336 32	14 8	25 6

*Distributed centers funded for FY 1998 additional capability are not yet reflected in the table due to pending acquisition.

Defense Research and Engineering Network (DREN)

The Defense Research and Engineering Network (DREN) is a robust, high-speed network that provides connectivity among the program's geographically dispersed user sites and shared resource centers. Approximately 1,000 of the 4,000 HPC users reside at the MSRC sites, while the remaining 75% are at remote locations. The program's networking initiative is supported by the Defense Information Systems Agency. DREN provides gateways to many existing military and civilian networks, allowing access to the program's resource centers from contractor and university facilities.

Recognizing that commercial industry is a much heavier investor in communications technology than is DoD, DREN has been implemented to take advantage of leading-edge commercial developments and the national information infrastructure. Accordingly, the DREN Intersite Service Contract (DISC) was awarded in July 1996. The contract allows the government to purchase high-speed network service to anywhere in the United States at bandwidths ranging from 1.5 megabits per second to 155 megabits per second (OC3), with upgrade potential to 2.4 gigabits per second (OC48) over the five-year life of the contract. Thirteen Interim DREN sites were transitioned to DISC in Fiscal Year 1997. An additional 47 government sites will be implemented in FY 1998, bringing the total to 60. Options to increase bandwidth at selected sites will also be executed to assure that network capacity keeps pace with user demands. In addition, wide-area classified networking is enabling support to classified processing requirements over DREN using high-speed Fastlane encryption technology.



Computational Technology Areas (CTAs)

The DoD HPCMP user community and the computational requirements that drive program resource decisions are organized around 10 CTAs. Each CTA has a designated leader who is a prominent DoD scientist or engineer working within the research disciplines included in the CTA. Table 3 describes the CTAs.

Table 3 — Computational Technology Areas

Computational Structural Mechanics CSM provides high-resolution, multidimensional modeling of materials and structures subjected to a broad range of static, dynamic, and impulsive loading conditions. Uses include effects of explosions on various facilities, underwater explosion and ship response, structural acoustics, structural analysis, propulsion systems, lethality and survivability (aircraft, ships, submarines, tanks), theater missile defense, and real-time, large-scale soldier and hardware in-the-loop vehicle dynamics.	**Signal/Image Processing** SIP provides for extraction and analysis of key information from various sensor outputs in real time. Sensors include sonor, radar, visible and infrared imagers, and signal intelligence and navigation assets. Uses include intelligence, surveillance and reconnaissance (ISR), avionics, communications, smart munitions, and electronic warfare. Functions include detecting, tracking, classifying, and recognizing targets in the midst of noise and jamming; generating high-resolution low-noise imagery; and the compression of imagery for communications and storage.
Computational Fluid Dynamics CFD provides the accurate numerical solution of the equations describing fluid and gas motion and fluid-dynamics research. Uses include the design of complex combustion and propulsion systems that are inaccessible or too costly to prototype; the dynamics of submarines, subsonic, transonic and supersonic air vehicles, pipe flows, air circulation, missiles, projectiles; and magnetohydrodynamics for advanced power systems and weapons effects.	**Forces Modeling and Simulation/C4I** FMS integrates high-speed command, control, communications, computers, and intelligence (C4I) systems to manage a battle space; provides large-scale simulations of complex military engagements to facilitate mission rehearsal/training, mission planning, and postmission analysis; and advances digital library technology for support of FMS/C4I research and development activities. Uses span the design, development, test, evaluation, and deployment of a variety of warfighting and training systems.
Computational Chemistry and Materials Science CCM provides prediction of basic properties of new chemical species and application of this molecular understanding to the development of advanced materials. Uses include design of new chemical compounds for fuels, lubricants, explosives, rocket propellants, and chemical defense agents. In addition, advanced modeling techniques are used to develop new high performance materials for electronics, advanced sensors, aircraft engines, semiconductor lasers, laser protection systems, advanced rocket engines components, and biomedical applications.	**Environmental Quality Modeling and Simulation** EQM provides high-resolution three-dimensional Navier-Stokes modeling of hydrodynamics and contaminant transport through air, ground, and aquatic ecosystems. Uses include stewardship and conservation of natural and cultural resources; prediction of chemical, and biochemical contaminant flows; design and operation of installation restoration, integrated management in support of environmental quality; noise evaluation and abatement; and water quality models.
Computational Electromagnetics and Acoustics CEA provides high-resolution multidimensional solutions of Maxwell's equations and acoustic wave equations. Uses include calculating fields about antenna arrays; signatures of tactical ground, air, sea, and space vehicles; the signature of buried munitions; performance/design factors for electromagnetic gun technology; high-power microwave performance; modeling of acoustic fields for surveillance and communication; seismic fields for mine detection; and acoustic shock waves of explosions for antipersonnel weapons.	**Computational Electronics and Nanoelectronics** CEN provides the design, modeling, and simulation of complex electronic devices, integrated circuits, and small components. Uses include lower costs, weights, size, and improved perform-ance of electronics through predictive high-fidelity modeling and simulation; analog/digital high-frequency circuit and device simulation and optimization; modeling and simulation of micro-electromechanical devices, micro-resonators, active and passive millimeter-wave circuits and structures; electronic/photonic interconnect and packaging analysis; and fault modeling.
Climate/Weather/Ocean Modeling and Simulation CWO provides the numerical simulation and forecast of the Earth's climate as well as oceanic and atmospheric variability. Uses include improved flight safety; search-and-rescue mission planning; propagation of weapons; aircraft and ship routing; antisubmarine and undersea warfare; enhanced capabilities in adverse weather; and the capability to predict magnetic storm-induced effects and outages on command, control, communications (C^3), surveillance, and navigation systems.	**Integrated Modeling and Test Environments** IMT applies high performance computing software tools and techniques with live tests and hardware-in-the-loop simulations for test and evaluation of DoD weapons, components, subsystems, and systems in virtual and composite virtual/real environments. Uses include digital scene generation, six degrees-of-freedom trajectory simulations, real-time test-data analysis and display systems for test control and evaluation, and high-fidelity engineering and closed-loop engagement models (one-on-one and few-on-few).

Common High Performance Computing Software Support Initiative (CHSSI)

CHSSI is building efficient, scalable, portable software codes, algorithms, tools, models, and simulations that run on a variety of HPC platforms and affect a wide number of S&T and DT&E scientists and engineers. CHSSI is organized around the 10 CTAs and involves expert teams working in close collaboration across government, industry, and academia. CHSSI teams include algorithm developers, applications specialists, computational scientists, computer scientists and engineers, and end users. Table 4 lists the current 43 CHSSI projects and principal investigators across the CTAs.

Table 4 — Common HPC Software Support Initiative Projects and Principal Investigators

Computational Technology Area	Project	Principal Investigator	Location
Computational Structural Mechanics	Small Deformation Structural Mechanics Large Deformation Structural Dynamics Scalable Algorithms for Shock Physics Structure-Medium Interaction Model	Gordon Everstine Raju Namburu Kent Kimsey Mark Emery	Naval Surface Warfare Center Army Waterways Experiment Station Army Research Laboratory Naval Research Laboratory
Computational Fluid Dynamics	FAST3D – Global Virtual-Cell Embedding Gridding COBALT – Unstructured Gridding FEFLO – Unstructured Gridding OVERSET – Chimera Gridding Zonal Navier Stokes – Block Structured Gridding Scalable NPARC	Jay Boris Bill Strang Bill Sandberg Bob Meakin Walter Sturek Jere Matty	Naval Research Laboratory Air Force Research Laboratory (Wright) Naval Research Laboratory Army – NASA Army Research Laboratory Arnold Engineering Development Center
Computational Chemistry and Materials Science	Car-Parinello Methods for Solids Quantum Chemistry Tight-Binding Molecular Dynamics Classical Molecular Dynamics	D.J. Singh Jerry Boatz D.A. Papaconstantopoulos Ruth Pachter	Air Force Research Laboratory (Wright) Air Force Research Laboratory (Edwards) Naval Research Laboratory Air Force Research Laboratory (Wright)
Computational Electromagnetics and Acoustics	Automatic Target Recognition and Scene Generation Electromagnetic Interaction Code Spectral Domain Low Observable Component Design Synthetic Sensor Phenomenology for Fusion Time Domain Numeric Methods for HPC Platforms High Resolution Computational Electromagnetics and Acoustics Code Magnetohydrodynamic Code	Jeff Hughes Jay Rockway Kueichien Hill Tom Blalock Helen Wang Miguel Visbal Robert Peterkin	Air Force Research Laboratory (Wright) Naval SPAWARSYSCEN, San Diego Air Force Research Laboratory (Wright) MSIC/Defense Intelligence Agency Naval Air Weapons Center (China Lake) Air Force Research Laboratory (Wright) Air Force Research Laboratory (Phillips)
Climate/Weather/ Ocean Modeling and Simulation	Ocean Models with Domain Decomposition Scalable Global Weather Forecast System Global and Regional Wind Wave Modeling	Steve Piacsek Tom Rosmond Robert Jensen	Naval Research Laboratory Naval Research Laboratory Army Waterways Experiment Station
Signal/Image Processing	Radar Signal Processing Scalable Algorithms for Sonar Beamforming Synthetic Aperture Radar/Image Formation HPC Embedded Applications for Target Recognition Infrared/Optical Image Processing for Reconnaissance and Surveillance	Rich Linderman Bob Bernecky Chris Yerkes Cathy Deardorf Lynda Graceffo	Air Force Research Laboratory (Rome) Naval Undersea Weapons Center Naval SPAWARSYSCEN, San Diego Air Force Research Laboratory (Wright) Army Night Vision Laboratory
Forces Modeling and Simulation/C4I	Scalable HPC Environment for C4I (SHEC) Simulation Leveraged Acquisition Test & Evaluation Efficient Parallel Discrete Event Simulation for Analysis HPC Frameworks for Warming and Training Simulations	Guy Leonard Henry Ng Bill Smith Larry Peterson	Naval SPAWARSYSCEN, San Diego Naval Research Laboratory Naval Research Laboratory Naval SPAWARSYSCEN, San Diego
Environmental Quality Modeling and Simulation	Structured-Unstructured Modeling Resolved Transport Algorithm Scalable Parallel Implementation of DoD Groundwater Modeling System	Robert Bernard Mark Dortch Fred Tracy	Army Waterways Experiment Station Army Waterways Experiment Station Army Waterways Experiment Station
Computational Electronics and Nanoelectronics	Scale Algorithms for Dynamic Nonlinear Simulations Power Electronics Simulation Parallel Very High Speed Integrated Circuit Hardware Description Language Simulation Electromagnetic Solvers for High Frequency Design	Dave Rhodes Robert Pastore John Hines Leo DiDominico	Army Comm and Electronics RDE Center Army Intelligent Electronic Warfare Center Air Force Research Laboratory (Wright) Army Research Laboratory
Integrated Modeling and Test Environments	Real Time Synthetic Test Environment Representation High Fidelity Physics Based Models for Testing Simulation Based Design and Test Technology	Harry Heckathorn Joel Mozer Andrew Mark	Naval Research Laboratory Air Force Research Laboratory (Phillips) Army Research Laboratory

DoD Challenge Projects

Beginning in FY 1997, the HPCMP began allocating 20% of the total computing resources to support very large, computationally intensive projects. These projects are selected annually based on proposals that are competitively reviewed and recommended by a peer review panel. This panel, which includes experts from outside DoD, reviews each proposal based on priority military needs, scientific merit, and potential for progress. Table 5 lists the FY 1998 challenge projects.

Table 5 — Fiscal Year 1998 DoD Challenge Projects

Primary CTA	Project	Organization	HPC System(s)
CSM	Development of Standards for Stand-Off Distance and Blast Walls for Force Protection	Army Waterways Experiment Station	IBM SP Cray T3E
CSM	Mine Plow Simulation by Smoothed Discrete Element Modeling	Army Waterways Experiment Station	Cray T3E IBM SP
CSM	Multistory Building Structural Response from Water Tamped Explosions	Army Waterways Experiment Station	IBM SP Cray T90 Cray T3E
CSM	Modeling of Complex Projectile-Target Interactions	Army Research Laboratory	Cray T90 Cray J90 Cray Origin 2000
CFD	Analysis of Jet Interaction Phenomena for the THAAD Interceptor	Army Space Missile Defense Command	Cray T90 Cray Origin 2000
CFD	Applied CFD in Support of Aircraft-Store Compatibility and Weapons Integration	Air Force Development Test Center	Cray Origin 2000 Cray T3E
CFD	Automatic Aerodynamic Design for Complete Aircraft Configurations Using an Adjoint Based Multiblock Method	Air Force Office of Scientific Research	Cray Origin 2000 Cray T3E
CFD	Parallel Simulations of Flow-Structure Interactions	Office of Naval Research	IBM SP Cray T3E
CFD	Parallel Simulations of Reacting Turbulent Two-Phase Flows	Army Research Office	Cray Origin 2000 Cray T3E
CFD	Simulation of Explosions for Counter-Proliferation and Counter-Terrorism Scenarios	Defense Special Weapons Agency	Cray Origin 2000 Cray T3E
CFD	Time-Domain Computational Ship Hydrodynamics	Office of Naval Research	TMC CM-5 Cray T90 IBM SP Cray Origin 2000 Cray T3E
CFD	Unsteady Hydrodynamics of the Maneuvering Submarine	Office of Naval Research	Origin 2000 Cray T3E
CCM	Dynamical Response of Low Dimensional Materials	Naval Research Laboratory	TMC CM-5
CCM	New Materials Design	Air Force Phillips Laboratory Air Force Office of Scientific Research	Cray T90 Cray Origin 2000 IBM SP
CCM	Theoretical Investigation of Gun Tube Erosion Related Requirement	Army Research Laboratory	SGI PCA Cray Origin 2000 Cray T3E
CEA	Airborne Laser Laboratory Challenge Project	Air Force Research Laboratory	Cray T3E IBM SP
CEA	B-1B Radar Cross-Section Prediction	Air Force Research Laboratory	IBM SP Cray Origin 2000
CEA	Computational Assisted Development of High Temperature Structural Materials	Air Force Research Laboratory Air Force Office of Scientific Research	IBM SP Cray Origin 2000 Cray T3E
CEA	Virtual Prototyping of RF Weapons	Air Force Research Laboratory	Cray T90 IBM SP
CWO	Global and Basin-Scale Ocean Modeling and Prediction	Naval Research Laboratory	Cray T3E
EQM	Quantification of the Impacts of Subsurface Heterogeneity on Military Site Cleanup	Army Waterways Experiment Station	IBM SP TMC CM-5 Cray T3E
CEN	Atomistic Simulation of MEMS Devices via the Coupling of Length Scales	Naval Research Laboratory	IBM SP
CEN	Quantum Simulation	Defense Advanced Research Projects Agency	Cray T3E

Success Stories

LISTING

Success Stories — Listing

Computational Structural Mechanics

Computational Fluid Dynamics

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61 Parallel Flow Simulations for Appended Submarines with Rotating Propulsors — R. Pankajakshan and W.R. Briley

62 Turbulent Nonlinear Free-Surface Wakes for a Combatant — E.P. Rood, D.G. Dommermuth, E. Paterson, F. Stern, and D.K.P. Yue

63 Second-Order Reynolds Stress Turbulence Modeling of Three-Dimensional Oblique Supersonic Injection — C.F. Chenault and P.S. Beran

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Computational Chemistry and Materials Science

Computational Electromagnetics and Acoustics

Climate/Weather/Ocean Modeling

Signal/Image Processing

Forces Modeling and Simulation/C4I

Environmental Quality Modeling and Simulation

Computational Electronics and Nanoelectronics

Integrated Modeling and Test Environment

SUCCESS STORIES

Computational Structural Mechanics

Computational Structural Mechanics (CSM) addresses high-resolution, multidimensional modeling of materials and structures subjected to a broad range of loading conditions. Contributions to DoD mission success from high performance computing applications in CSM span a number of DoD Joint Warfighting Capability Objectives, including Precision Force, Joint Readiness and Logistics, Military Operations in Urban Terrain, and Joint Countermine.

The CSM stories that follow have been selected to illustrate the paramount role that HPC plays, in both the development of advanced technologies and the evaluation of various design alternatives, as an integral component of DoD's RDT&E programs. The grand challenge aspect of CSM is illustrated in the success story that discusses the modeling of airblast loading and multistory building response to develop protection standards for terrorist threats. Examples of state-of-the-art CSM applications include, among others, finite-element transient shock analysis for shock-qualification trials, modeling the shape effects of hypervelocity projectiles by using the smooth particle hydrodynamics method, three-dimensional fluid-structure interactions for modeling parachute and airdrop systems, aeroelastic analysis of flexible aircraft structures, and soil-structure interaction analysis of explosion-induced ground-shock propagation. Several of the CSM success stories that follow are based on scalable computations and algorithms being addressed in the CSM computational technology area under the aegis of the DoD Common High Performance Computing Software Support Initiative.

Kent Kimsey
Army Research Laboratory
Aberdeen Proving Ground, MD
CTA Leader for CSM

Steady Aeroelasticity in the Transonic Regime

Lt. G.R. Andersen, U.S. Air Force
Air Force Research Laboratory, Wright-Patterson AFB, OH

HPC Computer Resource: Cray C90 [ASC MSRC]

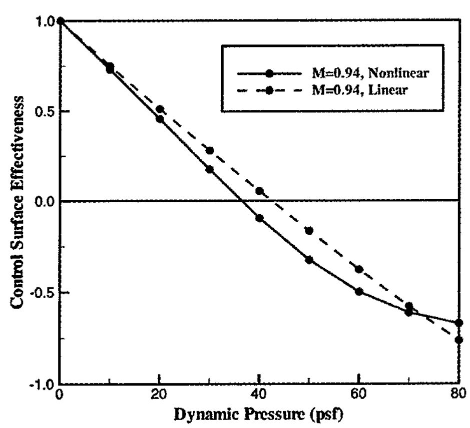
Research Objective: To develop accurate and efficient steady aeroelastic analysis and design capabilities for use in the automated preliminary design of flight vehicles, which include the effects of flow nonlinearities and structural flexibility in the transonic flight regime.

Methodology: Flow nonlinearities created by shocks in transonic flow are included in an aeroelastic analysis of the rolling maneuver performance of a fighter wing by using the CAP-TSD code to solve the transonic small disturbance equation. Pressure distributions and parameters pertinent to roll performance, including rolling moment coefficients, control surface effectiveness values, and control surface reversal dynamics pressures, were obtained from the CAP-TSD code and were compared to results obtained from linear methods.

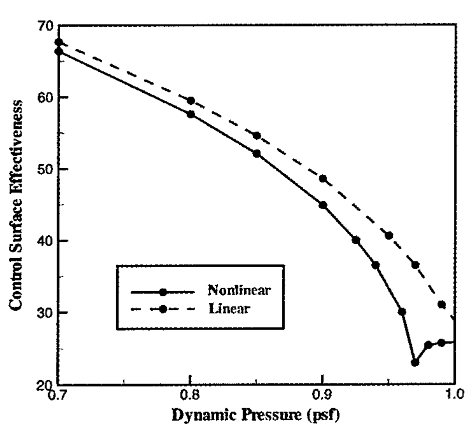
Results: The figures illustrate the effects of including flow nonlinearities in the steady aeroelastic analysis of the fighter wing. The top graph shows the differences between linear and nonlinear predictions of control surface effectiveness values at a Mach number of 0.94. The bottom graph demonstrates the significant effect of including flow nonlinearities in the prediction of control surface reversal dynamic pressures. The right-hand image shows the resultant pressure distribution acting on the wing due to the presence of shocks located on the surface of the wing.

Significance: The results of this study indicate the importance of including flow nonlinearities in the aeroelastic analysis of flexible aircraft structures. Differences between linear and nonlinear predictions of control surface reversal dynamic pressures of up to 38% were found. This research clearly suggests that linear techniques alone are not sufficient in the design of high performance aircraft that operate in the transonic flight regime.

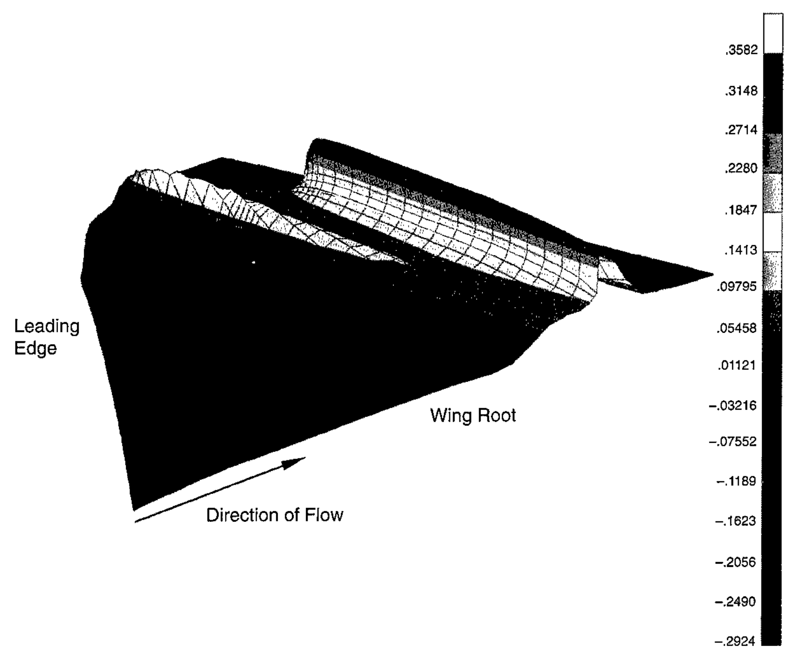
JWCO: Information Superiority



Control surface effectiveness values at Mach 0.94



Variation of control surface reversal dynamic pressures with Mach number



Resultant pressure coefficient distribution for nonlinear aeroelastic analysis at Mach 0.94

Effects of Water Tamping on Airblast from Near-Surface Cylindrical Charges

J.P. Balsara, R.R. Namburu, B. Armstrong, and T.L. Bevins
Army Engineer Waterways Experiment Station, Vicksburg, MS

HPC Computer Resource: Cray T3E [CEWES and NAVO MSRCs]

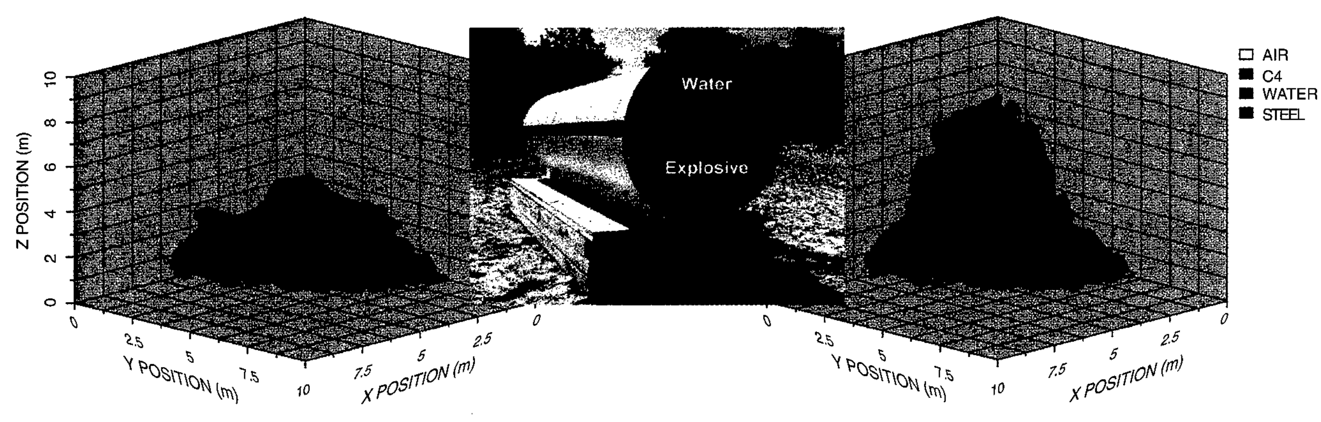
Research Objective: To investigate the effects of water tamping on the airblast characteristics from near-surface cylindrical charges.

Methodology: Experience with recent terrorist attacks indicates that current analytical prediction methods are inadequate for characterizing and understanding complex charge geometries and tamping effects. The problem involves modeling of high-explosive initiation, detonation, rupture, fragmentation, and blast-wave propagation. To model these phenomena, a three-dimensional simulation may require solving millions of nonlinear equations. CHSSI scalable software PCTH along with constitutive models based on material property experiments was used on a Cray T3E to perform the simulations. PCTH is a two-step explicit solution scheme that marches in time and uses message passing interfaces to communicate between processors.

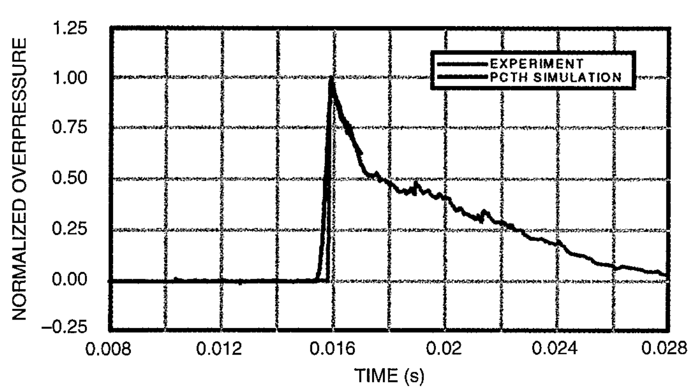
Results: The numerical simulations have provided a wealth of information necessary to understand asymmetry of the blast pressures and the effects of water tamping from near-surface cylindrical charges. Numerical simulations and the results of large-scale experiments are in excellent agreement. The computational domain is discretized using 32 million finite-volume cells to adequately model the problem. Simulations are performed on a Cray T3E using 128 processors and 150 Mbytes of memory on each processor. Linear scalability of the PCTH software is observed on the Cray T3E.

Significance: Because of the complex nature of the phenomena, parametric studies using numerical modeling are the only way to understand tamping effects for near-surface cylindrical explosions. These studies will assist DoD in evaluating realistic threats from near-surface explosions and, in turn, will assist in developing protective standards against terrorist threats.

JWCO: Combat Identification, Military Operations in Urban Terrain, Joint Readiness and Logistics, Joint Countermine



Tamped and untamped explosions depicting detonation products and water at 1.3 ms



Comparison with experimental results

Load Capacity of an Assembly via Structural Analysis

R.P. Garcia and D. Trinh
Tank-Automotive Research, Development, and Engineering Center, Warren, MI

HPC Computer Resource: SGI PCA [TARDEC DC]

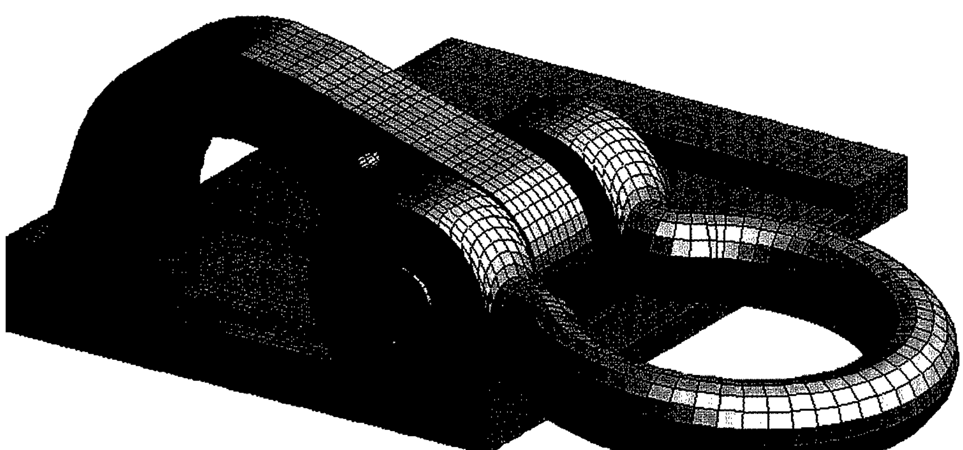
Research Objective: To determine the structural load carrying capacity of the Abrams main battle tank rail transport tie-down system by using a proposed new shackle design. This system comprises a lifting eye, a shackle, and a shackle pin.

Methodology: The simulation conducted was a series of finite-element structural analyses. The three-dimensional structural model of the rail tie-down system was constructed using a commercial software package called PATRAN, which has 86,000 degrees of freedom. The model was analyzed by using a commercial finite-element solver called ABAQUS. This solution algorithm used two CPUs from an SGI R10000 PCA. A typical analysis run consumed 16 CPU hours but required 2 Gbytes of memory to solve in-core. The analyses were nonlinear static simulations incorporating deformable contact between each of the tie-down system components. Two different material properties were used for the shackle/pin, and seven different loading magnitudes were applied. A total of 800 CPU hours were used on this project.

Results: This analysis study showed that the rail transport tie-down system with the proposed new shackle design is capable of handling 2.5 gravitational units based on a vehicle weight of 70 tons. This is exactly the capacity of the system using the current Abrams shackle, which is the one from the Bradley vehicle. If the material properties of the shackle and pin are greater than the lifting eye material properties, the weakest point in the system is the lifting eye. If the material properties of all components are equal, the pin and the shackle are the weak spots.

Significance: Because the tie-down system using the proposed new shackle design is just as structurally capable as the current system, no procurement of new shackles for the Abrams fleet is foreseen. Also, the lifting eye attachment does not require retrofit into the Abrams fleet as long as material properties are similar between the lifting eye and the shackle and pin. Any retrofit to the fielded Abrams system would not only cost time and money, especially at a time when funding is being reduced, but would have the possibility of taking out of service a portion of the main battle tank fleet, which would affect combat readiness.

JWCO: Joint Readiness and Logistics



Finite-element model of Abrams lifting eye, shackle, and pin system

Large-scale Particle Simulation Reveals Critical Soil Deformation Mechanisms During Mine Clearing

D.A. Horner, J.F. Peters, and A.R. Carrillo
Army Engineer Waterways Experiment Station, Vicksburg, MS

HPC Computer Resource: SGI PCA and Cray C90 [CEWES MSRC]

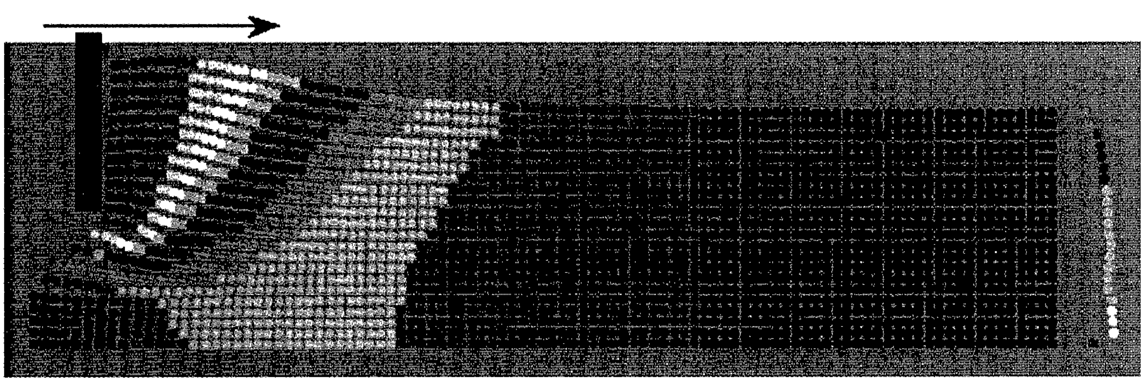
Research Objective: To develop the numerical capability to provide realistic off-road mobility modeling. In particular, the primary objective is to develop models to predict behavior of soils subject to large discontinuous loadings from vehicular traffic. The projected benefit of this research is to assist in reducing the life-cycle cost of military vehicles by supplementing the existing field experimental program with numerical simulations so as to reduce the number of live experiments to be performed during the design phase of a vehicle.

Methodology: The discrete element method (DEM) provides a means of simulating soil reactions during laboratory plowing experiments. The DEM idealizes granular media as individual particles or aggregates whose interactions are controlled by simple constitutive relationships for interparticle contacts. DEM as configured is not feasible for full-scale simulations, but it can provide micromechanical data to formulate a continuum mechanics model that will be suitable for vehicle simulations.

Results: An experiment of 65,000 particles was shown to accurately simulate a laboratory experiment in which there was a nearly one-to-one correspondence between the performance of simulated particles and actual sand grains. Micromechanical data from selected material points were used to formulate a continuum model based on the concept of a smoothed particle. A smoothed particle model replicated the plow experiment using only 2200 particles. Of vital importance, the general issue of how micromechanical quantities evolve during large deformations was resolved. Thus, the smoothed particle model is scalable to field problems, which implies that a comparably sized computation could replace a DEM simulation having billions of particles.

Significance: The numerical models are valuable tools in fielding new vehicles and vehicle mounted weapon systems from concept to prototype. One of the most critical missing elements is a robust continuum-based model of the soil that will simulate large deformations in the soil imposed by military vehicles. The research described will fill the critical technology gap.

JWCO: Joint Readiness and Logistics, Joint Countermine



Plow experiment using smoothed (continuum) particle model representing 2200 particles to replicate a DEM simulation having 65,000 particles

Shock Analysis of SEAWOLF Hull Penetration Test Items

R.C. Ingler, J.P. Murray, and P.A. Mantz
Naval Surface Warfare Center, Chesapeake, VA

HPC Computer Resource: Cray C90 [CEWES MSRC]

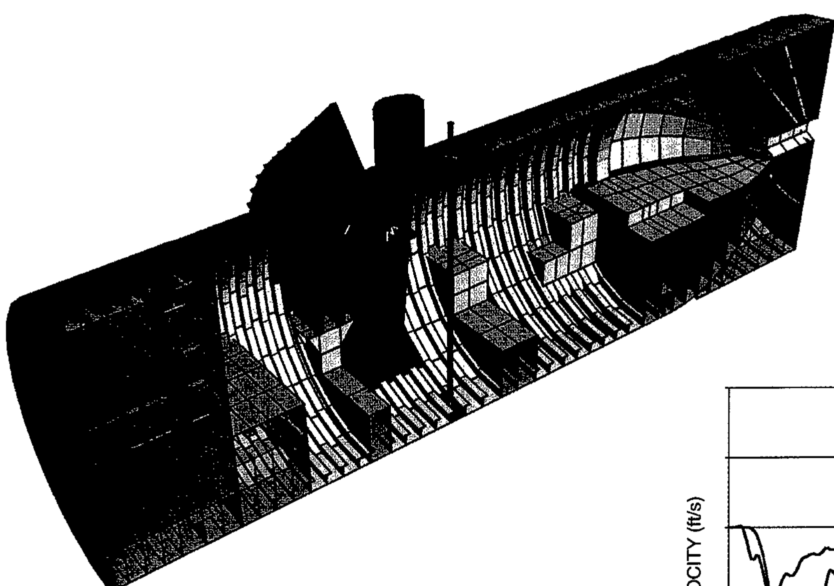
Research Objective: To evaluate a series of underwater explosion shock qualification test geometries for SEAWOLF-class submarine hull penetration test items installed on a large shock test vehicle, in order to develop an optimized test plan for a multimillion dollar submarine weapons delivery system shock qualification trial.

Methodology: A finite-element model of the Navy's large shock test vehicle and several SEAWOLF hull penetration test items installed in the vehicle for shock qualification were developed in CSA/NASTRAN. Equipment items represented included the logistic escape trunk (LET), the bridge access trunk (BAT), periscope, and internal auxiliary launcher (IAL). Transient shock analyses were performed to assess the severity of 23 qualification tests and several alternative tests that are aimed at satisfying the design and test requirements for multiple items simultaneously. This approach ultimately will enable the programmatic requirements to be satisfied with fewer overall tests.

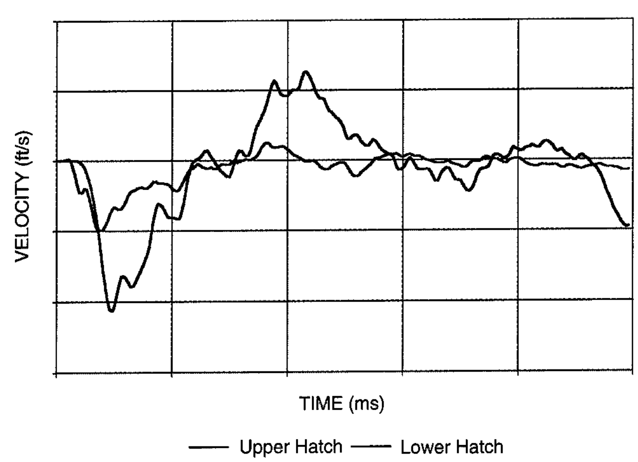
Results: Peak velocity responses, time histories, and trunk rocking motions were compared for 23 dedicated qualification tests and 24 candidate alternative tests. Assessment of the results allowed for the selection of an optimized test plan consisting of a total of 10 geometries that will successfully accomplish shock qualification requirements for each of the test items.

Significance: As a result of the rapid turnaround of the high performance computer predictions, an optimized test plan was developed in a timely manner impacting the implementation of the shock qualification trial plan. The estimated cost savings to the Navy brought about by this significant reduction in the required number of tests (from 23 to 10) is between 3 to 4 million dollars.

JWCO: Joint Readiness and Logistics



Cutaway view of finite-element model of vehicle and test components



Computed rocking motion of the logistic escape trunk

Scalable Computations in Penetration Mechanics

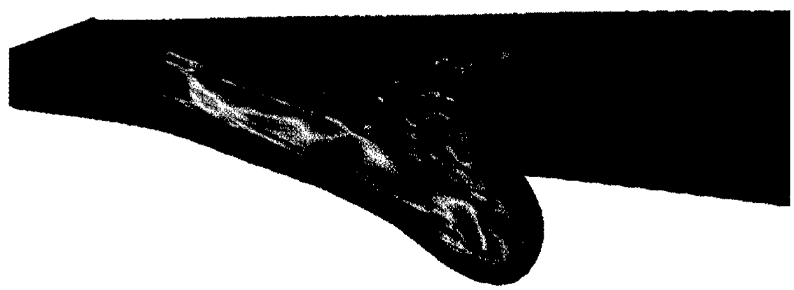
K.D. Kimsey and S.J. Schraml
Army Research Laboratory, Aberdeen Proving Ground, MD
E.S. Hertel
Sandia National Laboratories, Albuquerque, NM

HPC Computer Resource: SGI PCA [ARL MSRC and TARDEC DC], SGI Origin 2000 [ARL and ASC MSRC], and IBM SP [ASC MSRC]

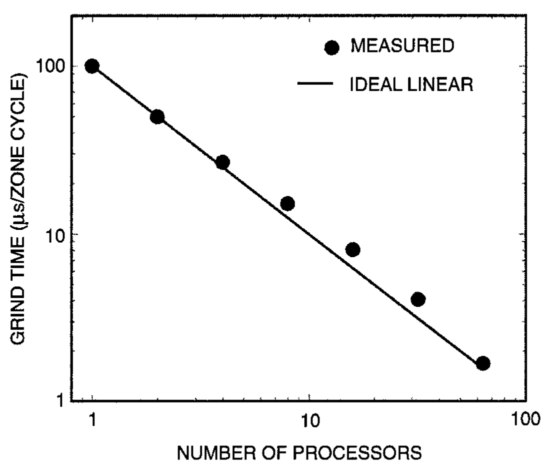
Research Objective: To develop, under a joint DoD/DOE CHSSI project, a suite of scalable shock physics software using advanced numerical methods coupled with advanced material models to model the nonlinear behavior of materials subjected to large deformations under high strain rate loading; to demonstrate that the shock physics software performs efficiently on a range of DoD scalable HPC platforms; to demonstrate the design utility of the scalable software with scalable demonstration simulations; and to integrate scalable shock physics application software into DoD programs.

Methodology: The computational methodology is based on the Eulerian finite-volume method. CTH is an Eulerian finite-volume code for modeling solid dynamics problems involving shock-wave propagation, multiple materials, and large deformations in one, two, and three dimensions. A two-step solution scheme—a Lagrangian step followed by a remap step—is used. A single program multiple data (SPMD) paradigm with explicit message passing between computational subdomains is used to map the global computational domain onto scalable architectures.

Results: Scalability studies were conducted on distributed memory, symmetric multiple processor and distributed, shared-memory architectures. Scalable performance of the message passing code was measured by the "grind time," which is the average CPU time required for the code to update all flow-field variables for one computational cell in a given time increment (cycle). Three-dimensional (3-D) impact simulations maintained a constant number of cells on each processor as the number of processors was increased. The largest problem studied comprised 25 million cells. The two figures show predicted pressure contours for a long rod impact (top) and the scalable performance of the message passing code on the IBM SP system (bottom).



Long rod penetration with combined yaw and obliquity. Rod colored by pressure contours (blue, low pressure; red, high pressure).



Scalable performance on the IBM SP. The blue line shows the theoretical scalable performance; red markers depict measured performance on the IBM SP.

Significance: Terminal ballistics simulations play a paramount role in the concept evaluation process as well as the research and development phases of enhancing the overall survivability and lethality of armored ground combat vehicles. Memory and CPU requirements delineate the HPC resources for large-scale terminal ballistics simulations. Doubling the number of cells in each coordinate direction by halving the characteristic cell length increases the memory requirement by a factor of 8 and halves the time step. The design utility of large-scale terminal ballistics simulations is derived from the ability to conduct a myriad of 3-D parametric studies as an integral component of armor and armaments R&D programs.

JWCO: Precision Force

Shape Effects of Hypervelocity Projectiles on the Damage of Laminate Composite Perforation

D.F. Medina and J.K. Chen
Air Force Research Laboratory, Kirtland AFB, NM

HPC Computer Resource: Cray C90 [CEWES MSRC]

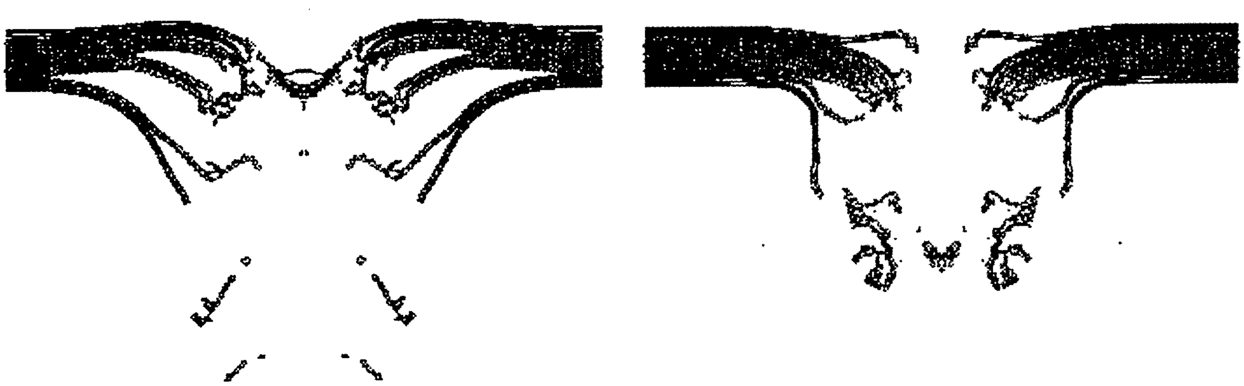
Research Objective: To investigate the response of B/Al composite laminates subjected to high-intensity loading by using a numerical technique known as smooth particle hydrodynamics (SPH) together with a micromechanics model.

Methodology: Numerical models of two different lay-ups, [02/902]s and [02/902]s, were generated in which the individual fibers and matrix were treated as individual materials. The lay-ups were impacted with projectiles differing in shape (circular and square with L/D = 1, 1/4 and 4) and impact speed (2 to 5 km/s). Application of this Lagrangian SPH technique is new to the analysis of composites. It was selected because of its ability to capture the complex phenomena resulting from high-velocity impact on composite laminates such as global deformation, local indentation, bulging, matrix cracking, delamination, and fragmentation. These high-strain phenomena are accommodated by SPH without the numerical problems characteristic of grid-based techniques such as mesh entanglement and distortion.

Results: The resulting calculations demonstrated detailed damage phenomena, which differed from each other as a function of differing impact velocities and projectile shape. Damage was assessed by the diameter of the damaged zone (maximum radius of delamination and bending) and perforation hole radius.

Significance: The superior characteristics of high stiffness- and strength-to-weight ratios of advanced composites have been the primary reasons for their application in space assets. For this reason, it is imperative that composite response to hypervelocity impacts of the type encountered in a space environment be understood and predicted. However, the numerical modeling of such complex material continues to be challenging. For this reason, conventional macromechanics composite models generally do not distinguish individual responses of the composite constituents. The introduction of the SPH technique together with the micromechanics model into the composite modeling field has provided a method to capture the complex perforation and damage progression resulting from high velocity impacts.

JWCO: Precision Force



Damage in the [02/902]s laminate impacted by the flat rectangular rod (h/w = 0.25) (left) and a thick rectangular rod (h/w = 4.0) (right) at 4.0 km/s and 3.5 ms

Simulation of Damage to a Multistory Building from a Terrorist Bomb

R.R. Namburu, J.P. Balsara, T.L. Bevins, and J.T. Baylot
Army Engineer Waterways Experiment Station, Vicksburg, MS

HPC Computer Resource: Cray T3E [CEWES MSRC]

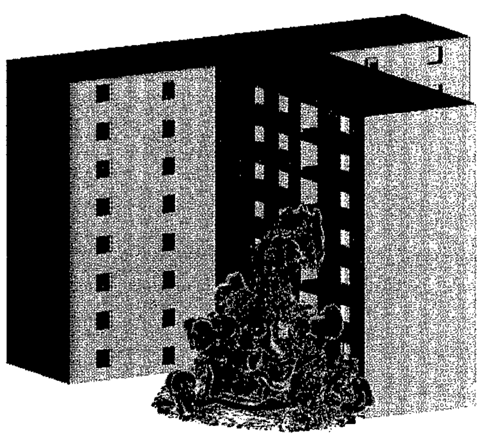
Research Objective: The threat to our operational forces and facilities is posed by increasingly sophisticated terrorist weapons. The Services need to develop new technologies for designing or retrofitting military facilities to ensure their security and survivability against terrorist attacks from a wide spectrum of weapons. Our objective, therefore, was to develop a methodology capable of simulating the damage and failure mechanisms of multistory buildings due to airblast from terrorist bomb detonations.

Methodology: A multistory building is modeled to include interior walls, doorways, windows, and stairway landings so that detailed asymmetric airblast propagations and their complex reflections with building materials throughout the interior of the building can be predicted. Material constitutive models used are being fit to an extensive set of recommended material properties. The analysis was performed using CHSSI Eulerian explicit software CTH and Lagrangian software ParaDyn. Recent advances in hardware and software have made it possible to simulate blast propagation and nonlinear structural response, including damage, in sufficient detail.

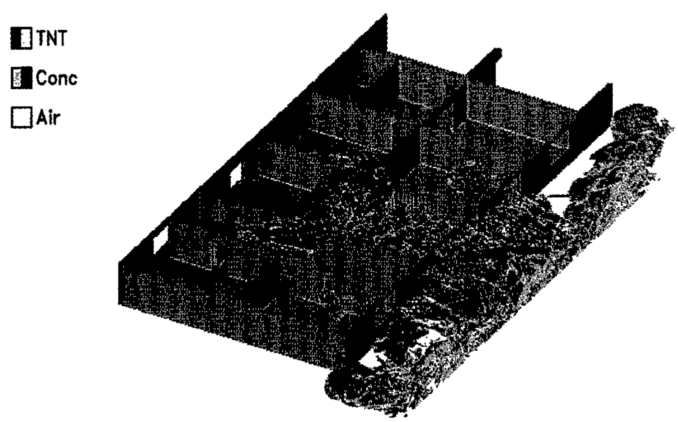
Results: To simulate a terrorist bomb detonation and blast wave propagation into the multistory building, the Eulerian domain is discretized using 85 million three-dimensional cells. The memory required to solve this problem is about 40 Gbytes. For structural damage analysis, the Lagrangian domain consisted of 162,192 loading surfaces and 27,994 tie-breaking nodes. The results provided an insight into the blast interaction with building components and blast effects on structural damage.

Significance: High-performance computing is the most cost-effective approach for developing protective standards for multistory buildings against terrorist threats. Simulations on scalable computers with experimentally validated numerical methodologies and material constitutive models will advance this technology and assist the Services in establishing protective standards for multistory buildings.

JWCO: Combat Identification, Military Operations in Urban Terrain, Joint Readiness and Logistics



Blast wave propagation and blast-structure interaction at 14 ms



Propagation of detonation products in the first floor at 12 ms

Large-Deformation Response of a Buried Hardened Structure Subjected to Explosion-induced Ground Shock

P.P. Papados and R.R. Namburu
Army Engineer Waterways Experiment Station, Vicksburg, MS

HPC Computer Resource: Cray T3E [CEWES MSRC]

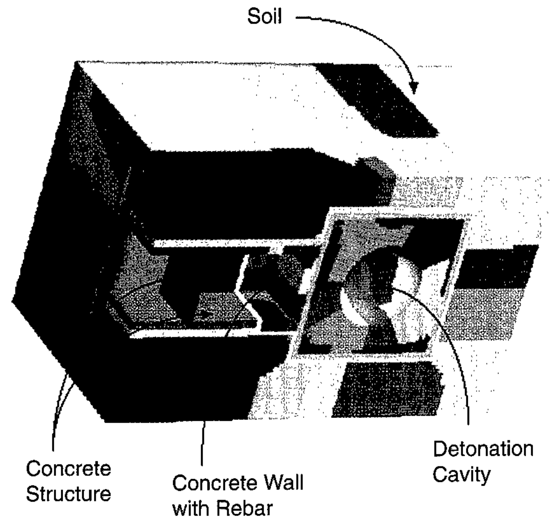
Research Objective: To investigate the survivability of hardened protective structures subjected to explosion-induced ground shock from modern conventional penetrating weapons threats.

Methodology: The immediate objective is to simulate damage of the primary wall of a buried structure subjected to loads resulting from the detonation of an explosion in soil adjacent to a structure. The ground shock propagation produced by the weapon detonation is altered by the presence of the structure. The resulting soil-structure interaction (SSI) produces a complex load on the buried structure. The simulations were performed using the CHSSI scalable, large deformation, explicit finite-element software ParaDyn using Waterways Experiment Station-validated material constitutive models for concrete and soil and 64 processors on a Cray T3E.

Results: The top figure shows the problem definition in which each color indicates the distribution of the problem geometry, including contact conditions, within each of the 64 processors. Very good linear scalability is observed for this nonlinear SSI problem. The center figure is the damage contour distribution on the primary wall of interest; a scale value of 2 indicates maximum damage. The bottom figure shows that, for this highly nonlinear problem, numerical computations indicate excellent agreement with the experimental results.

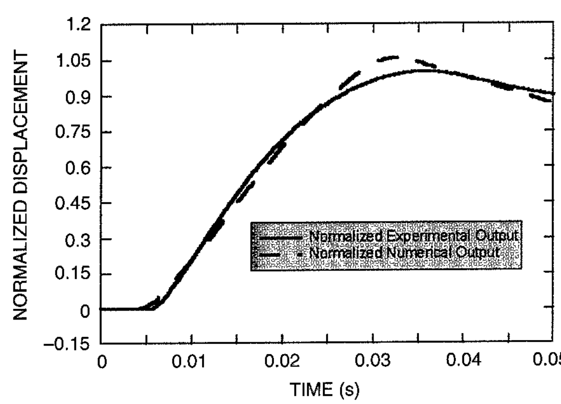
Significance: Experimentally validated numerical models are used to investigate the survivability of protective structures against explosion-induced ground shock. The methodology implemented in this study constitutes a significant advance in the numerical analysis of highly nonlinear SSI problems.

JWCO: Joint Readiness and Logistics, Joint Countermine



Quarter model of a buried concrete structure showing domain decomposition over 64 processors

Damage distribution of the reinforced concrete wall



Maximum structural deflection comparison between experiment and numerical simulation in the reinforced concrete wall

Computer-based Crash Worthiness Analysis of M113/BMP-2 Opposing Forces Surrogate Vehicle Turret

M.K. Pozolo
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HPC Computer Resource: SGI PCA [TARDEC DC]

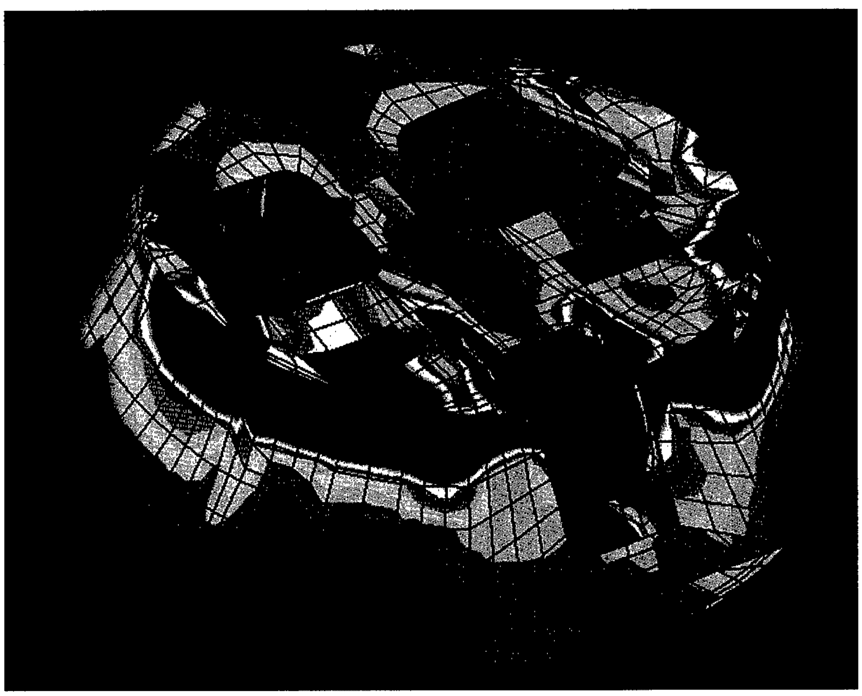
Research Objective: To determine what, if any, effect modifications to the roof and sidewall design would have on the crash worthiness of the M113/BMP-2 OSV turret.

Methodology: A three-dimensional, finite-element model of the M113/BMP-2 opposing forces surrogate vehicle (OSV) turret was created using the commercial software package MSC/PATRAN. The model had 13,440 degrees of freedom, and a nonlinear analysis was performed using the ABAQUS/Explicit dynamic finite-element program, an analysis module for transient dynamic applications that is especially suited for handling large deformations involving contact conditions between deforming bodies. Initial conditions applied to the M113/BMP-2 OSV turret model simulated a rollover of the vehicle onto the turret roof. This simulation was run on two CPUs from an SGI R10000 PCA.

Results: The results of the analysis showed that the turret redesign did not have a significant effect on the crash worthiness of the M113/BMP-2 OSV turret when subjected to a rollover scenario. The maximum deflection of the turret roof actually decreased on the driver side of the turret and increased only 1 to 2 inches on the curb side.

Significance: Using computer-based computational methods to analyze the crash worthiness of the OSV turret eliminated expensive and impractical field tests of the structure. The analysis was performed prior to production of the turrets and therefore would have flagged any design flaws before production runs started.

JWCO: Joint Readiness and Logistics



M113/BMP-2 OSV turret plastic equivalent strain contour plot showing deformation after 50 ms of simulated rollover

Fluid-Structure Interactions in Interior Ballistics

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HPC Computer Resource: TMC CM-5 [AHPCRC DC]

Research Objective: To develop numerical tools for the study of fluid-structure interaction phenomena that occur in interior ballistics, specifically within a solid propellant (SP) gun. The specific application is the study of the flow of hot gas between and around pieces of propellant within the combustion chamber of an SP gun. As the pieces of propellant are moved by the pressure forces of the gas, flow passages may be closed.

Methodology: The Navier-Stokes equations of compressible flow are discretized using a stabilized space-time finite-element formulation, which is capable of handling the changes in the shape of the gas domain caused by the motion of the propellant. To study the fluid-structure interaction problem, the fluid model is coupled to a numerical model of a deformable solid. The fluid mesh is updated within each time step using an advanced mesh update strategy. Three large linear equation systems are solved in each time step using iterative solution methods.

Results: A portion of the combustion chamber is being studied using experimental data for the pressure and temperature as boundary conditions. One piece of propellant is treated as movable and deformable. It is modeled alone and also with five other pieces of propellant, which are treated as rigid bodies fixed in space. The results are leading to an understanding of the motion of the propellant and its interaction with the gas.

Significance: A possible improvement to guns currently in the field is an increase in the amount of propellant in the rounds. In order to have a larger amount of propellant burn properly, the motion of the gas, and thus the motion of the propellant, must be understood. The results from this work are providing valuable insight into the interaction between the gas and the propellant during the firing cycle.

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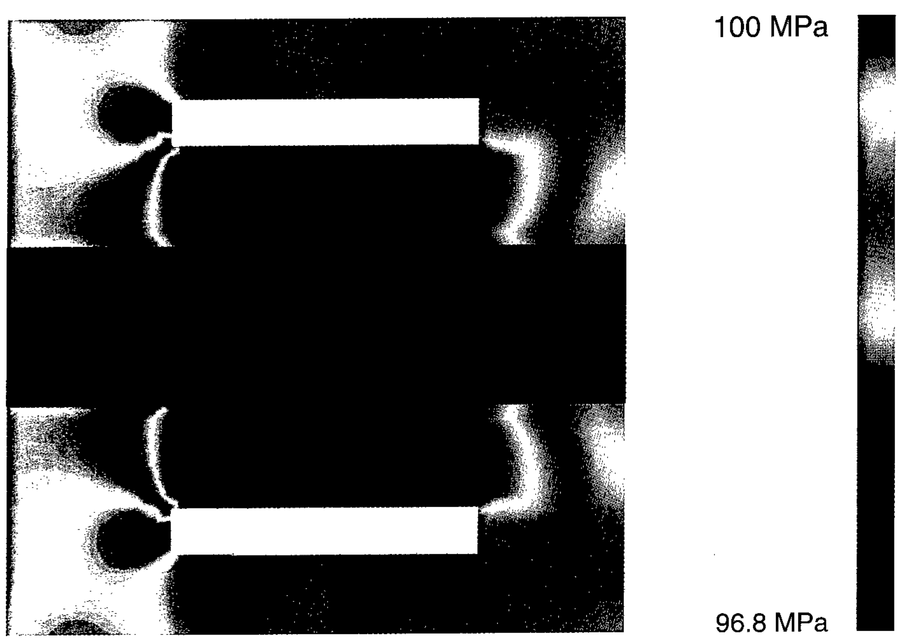

Gas pressure in a cross-section of the domain at one point during the firing cycle. The black region down the center is the projectile, and the white rectangles are propellant. Although the geometry is three-dimensional, the solution at this point in time is still symmetric. The presence of a little propellant affects the evolution of the pressure field, as can be seen in the figure where the lowest pressure is between the propellant and the projectile. The presence of more propellant should have an even greater effect.

Simulation of Parachute Fluid-Structure Interactions

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HPC Computer Resource: TMC CM-5 [AHPCRC DC]

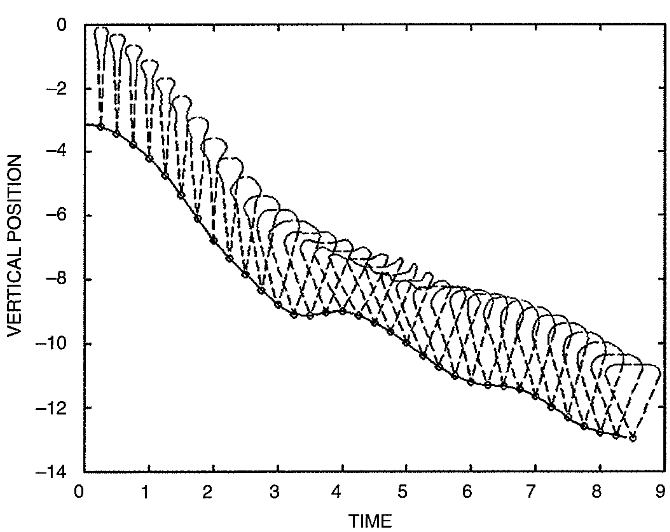
Research Objective: To establish numerical modeling methods for parachute design and development work. The techniques must be able to accurately predict the interactions between the parachute structural system and the surrounding flow field, which are dominant in most airdrop situations.

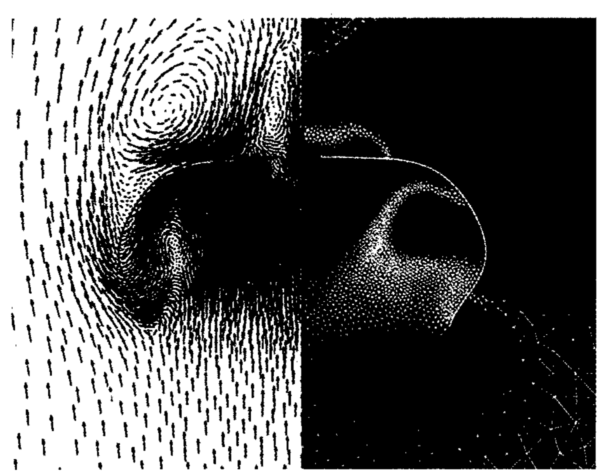
Methodology: The three-dimensional (3-D) Navier-Stokes equations for incompressible flow are discretized using a stabilized space-time finite-element formulation and with unstructured meshes for efficient meshing of arbitrary spatial domains. The structural dynamics equations of motion are solved using a finite-element formulation for a structure composed of membranes (canopy), cables (suspension lines), and concentrated masses (payload). The incompressible flow and the structural dynamics are numerically coupled along the canopy surface. An automatic mesh moving scheme (with occasional remeshing) is used to handle deformations in the spatial domain caused by parachute motions.

Results: These techniques are being developed for application to 3-D parachute fluid-structure interactions. The test problem depicted is for a coupled simulation of the opening of an axisymmetric parachute. The simulation captures important features of the inflations, such as peak opening forces and stresses, inflation times, and the overinflation of the canopy caused by wake recontact.

Significance: Parachutes and airdrop systems have been traditionally developed by time-consuming, costly, full-scale testing. The capability to use parallel computers to model and develop parachutes and airdrop systems will greatly reduce the time and cost of full-scale testing and assist in the optimization of new capabilities. Fluid-structure interactions are experienced at all stages of airdrop systems performance including initial deployment, inflation, terminal descent, and soft landing. These interactions must be accounted for to accurately model most parachute systems dynamics.

JWCO: Joint Readiness and Logistics





The figures show, for an axisymmetric simulation, the computed geometries and vertical position of the structural model at equally spaced instances in time throughout the computed inflation process. Also shown is a snapshot of the computed flowfield and unstructured mesh with the vector velocity field on the left and the unstructured mesh and computed pressure field (blue, low pressure; red, high pressure) on the right.

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Fluid-Structure Interactions in Interior Ballistics

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Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) is the accurate numerical solution of the equations describing fluid and gas motion. CFD encompasses nearly half of DoD HPC use and is applied to engineering design of DoD vehicles, facilities, and propulsion systems as well as for fundamental studies of fluid dynamics and turbulence. The CFD success stories that follow illustrate both Grand Challenge science and state-of-the-art engineering by some of DoD's top laboratories, academic partners, and industry partners. The stories show applications of a number of different generic approaches to "realistic CFD in very complex geometry." The success stories also include CFD coupled to complex physics. More than in the past, complex physics coupled to CFD tackled reactive flow modeling for increasingly realistic science and engineering problems. This year significant work was also undertaken in fundamental fluid dynamics including turbulence, where our understanding of complex fluid flow has been enabled by the world-class facilities and resources made available through the DoD HPC Modernization Program.

Complex geometry contributions include studies of the BQM-74 aerial target performance, the simulation of the Low Cost Autonomous Attack System dynamics, aerodynamic analysis of active control wings, extended range projectiles and parachute clusters, aerodynamic control of theater defense missiles using jet reaction controls, analysis of the Titan IV ignition overpressure including the surrounding launch stand and resulting side forces, turbulent free surface flow about high speed naval combatants, and the computational determination of external store carriage forces and moments. Reactive flow problems treated successfully include the design of an open detonation/open burn facility for the environmentally sound destruction of obsolete, demilitarized munitions, improved combustion control with coaxial jet systems, analysis of chemical oxygen-iodine laser propagation medium quality, missile exhaust plume phenomenology, and combustion of new high-energy fuels. Complex physics and CFD is also being extended to a number of multidisciplinary activities including development of a coupled CFD/CSM methodology to model the affects/results of potential terrorist attacks and contaminant transport modeling for defense against chemical and biological weapons attacks in urban environments. Fundamental fluid dynamic studies include using electricity and magnetism to control turbulence, a study of turbulent nonlinear free surface wakes, second-order Reynolds stress modeling for 3-D oblique supersonic injection, and a detailed determination of the shock-flame interaction mechanism responsible for the deflagration to detonation transition.

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CTA Leader for CFD

BQM-74 Target Aerodynamic Performance Analysis Support

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R. Meakin
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HPC Computer Resource: SGI PCA [NAWCAD DC]

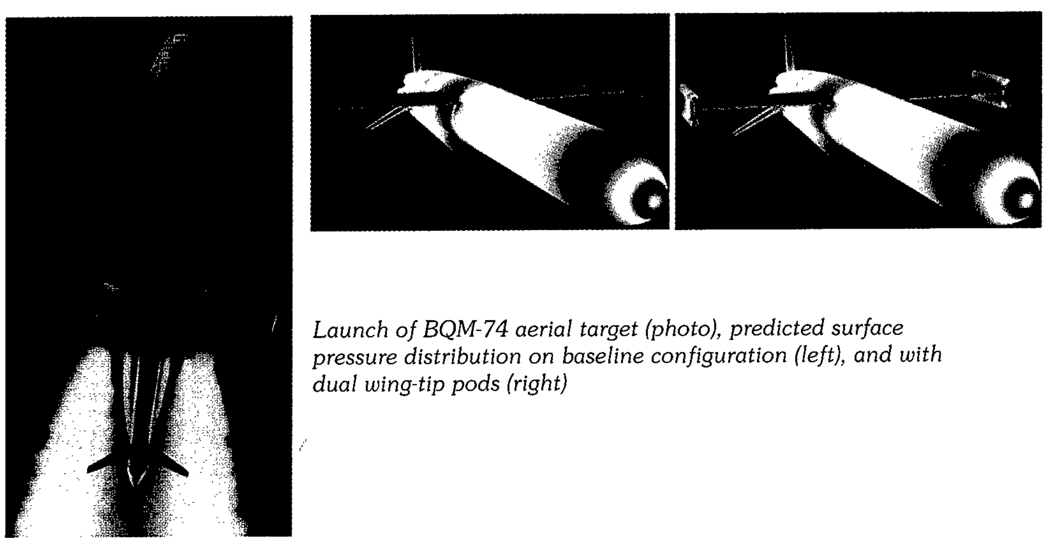
Research Objective: To demonstrate the utility of an overset grid approach in rapidly providing accurate performance data for modifications to existing Fleet vehicles. It is not uncommon for the U.S. Navy Fleet to require vehicle performance in roles beyond those anticipated in the initial design. In these instances, additional aerodynamic performance information is required to evaluate changes in vehicle performance and associated mission capabilities. The BQM-74 aerial target in which additional wing tip dual pods were added to the baseline configuration is a recent example of this. The new pods increase aerodynamic drag and affect mission range.

Methodology: The overset structured grid generation tools and flow solver software being developed through the CFD CHSSI projects were used in this work. The use of an overset grid approach is well-suited to this type of analysis. The existing overset grid system for the BQM-74 aerial target is easily modified to reflect the design change. Only the grid components associated with the change need to be replaced. All other grid components are completely reusable.

Results: The OVERFLOW-D code is used to simulate the steady viscous flow about the baseline and modified configurations of the BQM target (see figure). The increase in drag caused by the wing-tip-mounted pods is accurately predicted in the simulations.

Significance: Improved analysis capability of this type translates to reduced cost by reducing the need for expensive wind tunnel and flight tests. It is estimated that a savings of $100,000 to $300,000 in model fabrication and testing could be realized for applications such as the BQM target, with as much as a 6-month reduction in design cycle time.

JWCO: Precision Force



Launch of BQM-74 aerial target (photo), predicted surface pressure distribution on baseline configuration (left), and with dual wing-tip pods (right)

Simulation of LOCAAS Aerodynamics

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HPC Computer Resource: IBM SP [CEWES MSRC]

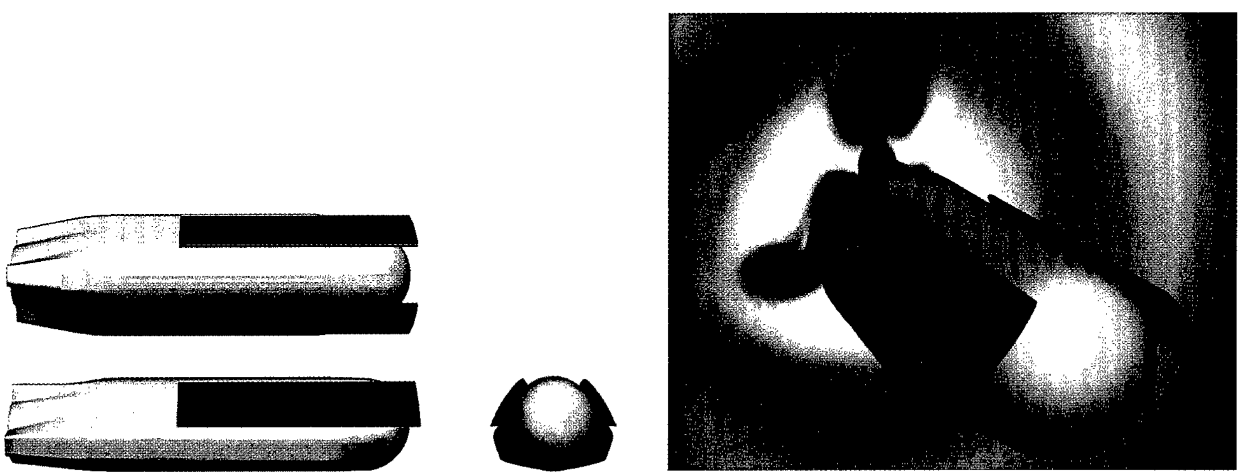
Research Objective: To define the unsteady aerodynamics that characterize the deployment flight profile of the Low Cost Autonomous Attack System (LOCAAS). The LOCAAS deployment sequence includes ejection from a dispenser, inflation of a ballute for speed reduction and flight stabilization, and deployment of wings and fins for autonomous controlled glide to intended targets. Computational analysis is being used to reduce costs and risks associated with anticipated flight test requirements.

Methodology: Overset structured grids are used to discretize the LOCAAS geometry. The approach is ideally suited to the LOCAAS flight profile. Grid components conform to the shape of the LOCAAS, facilitating resolution of the viscous boundary layer and important off-body aerodynamics. Grid components are allowed to move with six-degrees-of-freedom in response to applied and aerodynamic loads without the need for re-gridding. A scalable version of the OVERFLOW-D1 code has been developed and is being used to accomplish project objectives.

Results: An initial simulation result is presented here for a solitary LOCAAS (stowed configuration) in stable level flight (see figure). The computation was run using 32 nodes of an IBM SP.

Significance: This effort has dual objectives that involve evaluation of scalable CHSSI software and the aerodynamic performance of the Low Cost Autonomous Attack System. LOCAAS is in the advanced development phase. It is designed to provide the technology base for future low-cost laser radar sensor submunitions. This sensor technology provides increased cost-per-kill efficiencies through the ability of the sensor to detect, extract, and classify a variety of ground mobile and fixed targets.

JWCO: Precision Force



LOCAAS geometry in stowed configuration (left) and Mach field in stable level flight (right)

Aerodynamic Analysis of Active Control Wings

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L.J. Huttsell
Air Force Institute of Technology, Wright-Patterson Air Force Base, OH

HPC Computer Resource: Cray C90 and Cray Y-MP [CEWES MSRC]

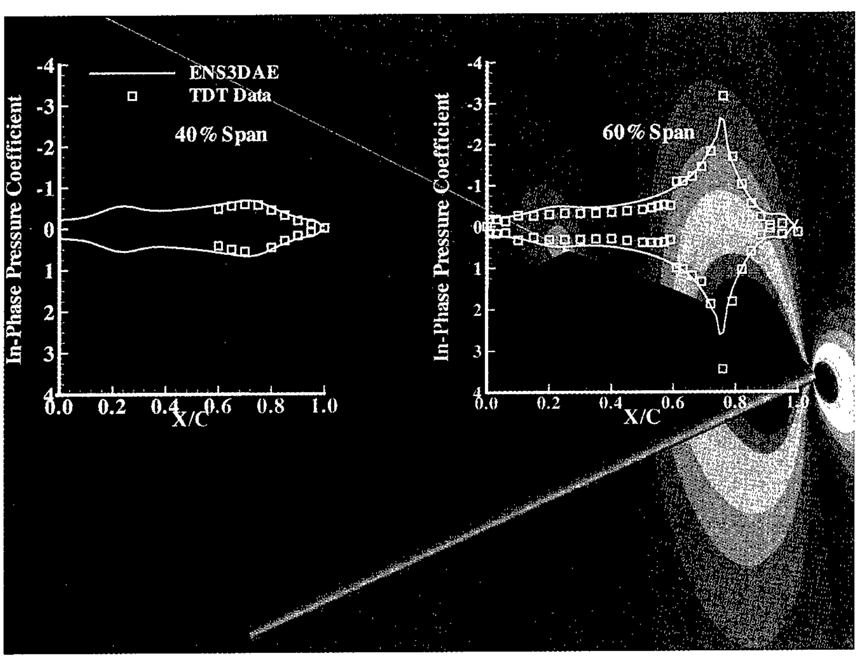
Research Objective: To develop an efficient simulation tool that can be used to predict the unsteady aerodynamic forces generated by actively deflected control surfaces. This technology will facilitate the development of accurate active control systems that are essential to the implementation of a Precision Force.

Methodology: A three-dimensional (3-D) viscous aeroelastic method (ENS3DAE) is used to compute the time-dependent aerodynamics about arbitrary vehicles. Nonlinear fluid dynamics equations are solved in conjunction with a structural deformation model to provide a high-fidelity simulation of the unsteady aerodynamic loads on the vehicle.

Results: The present application focuses on the aerodynamics of a wing with an oscillating control surface. The figure shows unsteady wing surface pressure distribution for a Navier-Stokes equation analysis of the wing with the aileron oscillating at 5 Hz. The flow conditions for this case are Mach 0.77, zero degrees angle-of-attack, and an aileron oscillation amplitude of two degrees. The component of the unsteady pressure that is in-phase with the aileron motion is compared with wind tunnel data. The 40% span location is just inboard of the aileron, while the 60% span station is at the spanwise center of the aileron. Comparison with unsteady experimental data is very good.

Significance: This calculation demonstrates that unsteady aerodynamic loads for wings with actively moving control surfaces can be accurately predicted. These data can be used in the development of active control laws to precisely maneuver and position flight vehicles. The ability to perform accurate simulations of this type will decrease acquisition time and cost by reducing the number of experiments and flight tests required to develop a weapons system.

JWCO: Precision Force



Pressure data on a rectangular wing model. The foreground compares theoretical and experimental unsteady pressure distributions. The wing geometry with the aileron deflected and the symmetry plane pressure distribution are shown in the background (blue: low pressure; red: high pressure).

CFD Analysis of Vertical Tail Buffet Flow Features

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HPC Computer Resource: IBM SP [MHPCC DC]

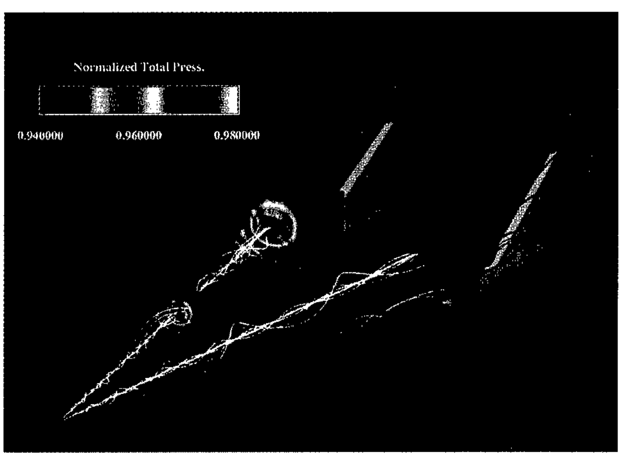
Research Objective: To provide efficient and accurate numerical predictions of vertical tail buffet loads during high angle-of-attack (AOA) flight conditions. The method is developed for design and trade study applications in lieu of expensive subscale testing. These calculations are intended to verify the validity of the prediction capability as well as provide greater insight to the flow phenomena present with this arrangement.

Methodology: The basic fluid dynamics analysis scheme is finite-difference-based and allows for first-order time-accurate solutions of the Reynolds-averaged Navier-Stokes equations. CFD analyses involving an enhanced version of the ENSAERO CFD code, including an overlapping multizone field grid methodology, was developed and used for this study. The analysis process allows for coupled fluid/structures/controls computations.

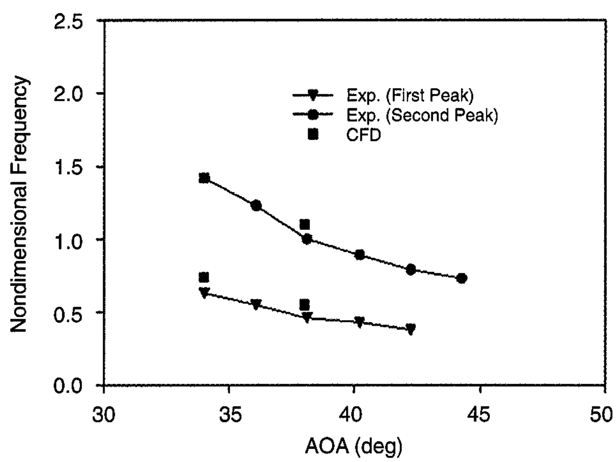
Results: Recent Navy/NASA/industry cooperative studies have focused on the production of a set of experimental data that characterize the flow field of high AOA tail buffet loads. In particular, one case included a 76-degree leading edge swept delta wing with twin-boom-attached vertical tails. The figure shows the delta-wing/vertical tail model that was used. This simplified geometry was chosen to isolate the vortex-tail interaction process. At moderate AOA, the wing main vortex is not burst, while a separate vortex forming over the vertical tail is burst. Time-accurate calculations for the wing and vertical tail geometry represent dominant frequencies very similar to experimentally measured values.

Significance: The results validated the computational method for such analysis. Subsequent analysis is now underway on a full-configuration flight test vehicle. The impact is in reducing the amount of ground and flight testing required to establish an adequate tail buffet environment, significantly increasing airframe fatigue life. Completion and validation of the model will provide savings of $0.5 to $1.0 M as the result of reduced ground and flight testing hours required. Additional benefits include approximately six months less time required to establish configuration modification effects during detailed design.

JWCO: Precision Force



Model of wing/tail configuration



Comparison of computed dominant frequencies of fluctuating surface pressures over the tail with experimental results as a function of angle of attack

Impingement of a Streamwise Vortex on a Control Surface

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HPC Computer Resource: Cray C90 [CEWES, NAVO, and ASC MSRCs] and IBM SP [ASC MSRC]

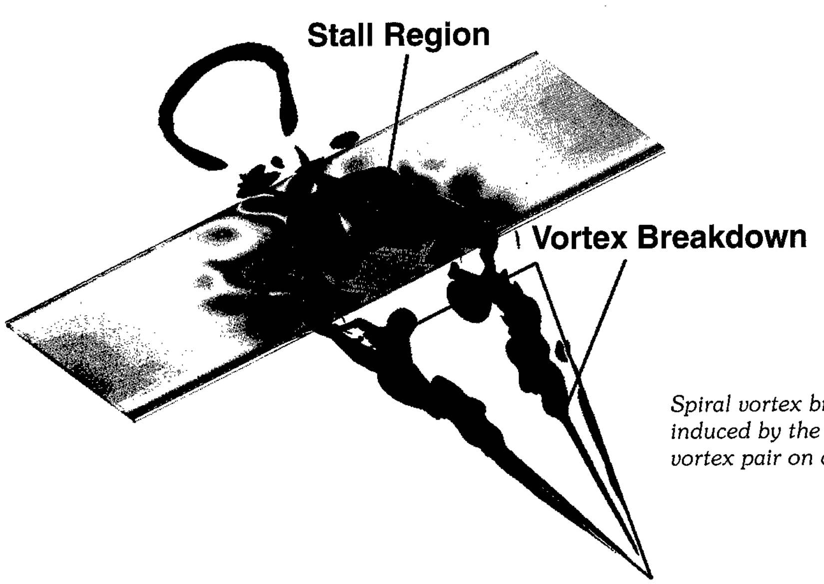
Research Objective: To examine in detail the flow structure arising when a streamwise vortex impinges directly on a downstream control surface. Modern fighter aircraft operating at high angles of attack exhibit the formation of a number of streamwise vortices that develop as a result of separation from leading edges. Although these vortices can be exploited for enhanced lift and maneuverability, they can also have detrimental effects when they interact with downstream control surfaces.

Methodology: The physical situation is modeled by simulating the impingement of a delta-wing vortex system on a plate located in the wake of the delta wing. The unsteady, three-dimensional, full Navier-Stokes equations are solved on an overset grid system using the implicit, approximately factored Beam-Warming algorithm. The resulting flow code (FDL3DI) has been fully vectorized and optimized for efficient operation on large vector processing machines. It has also been adapted to run on parallel platforms through a simple domain decomposition technique.

Results: Several principal flow elements were revealed as a result of these computations. These included spiral vortex breakdown over the wing induced by the presence of the plate, large-scale stall underneath the plate between the incoming vortex pair, and an outboard shallow separation region on the upper surface. A pronounced sensitivity of the breakdown location to the plate large scale stall region was also demonstrated for the first time. By exploiting this feature using active control techniques, alternate means for shifting the breakdown location or vortex trajectory may be possible.

Significance: The same aerodynamic phenomena that enhance the maneuverability and agility of high-performance aircraft can interact adversely with control surfaces, resulting in loss of control effectiveness, structural fatigue, and ultimately catastrophic failure of these components. A typical example of this is the phenomenon of tail buffet in twin-tailed aircraft. Improved understanding of these complex flows through computational simulation will allow for the development of new control techniques and aircraft designs to negate the adverse effects of these phenomena. This will result in reduced lifecycle costs for future aircraft and will extend the useful service life of the existing fleet.

JWCO: Joint Readiness and Logistics



Spiral vortex breakdown and large-scale stall induced by the impingement of a delta-wing vortex pair on a downstream surface

Control Surface Reversal of an Aeroelastic Wing

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HPC Computer Resource: Cray C90 [ASC MSRC]

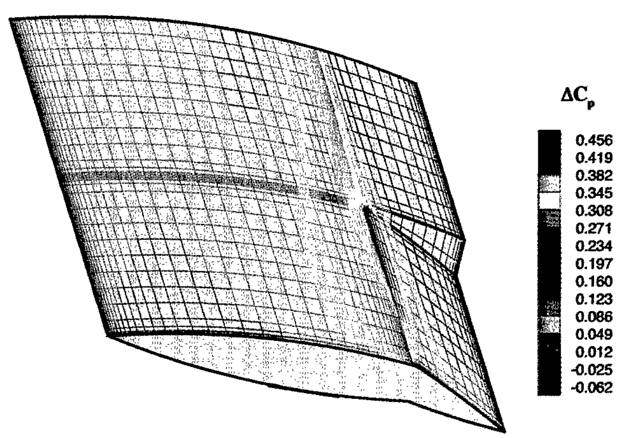
Research Objective: To validate the predictive ability of the high-fidelity ENS3DAE multiple-zone three-dimensional Euler/Navier-Stokes algorithm for control-surface reversal of an aeroelastic wing at subsonic and transonic speeds, and to evaluate changes in flowfield behavior associated with flap deflection in the transonic regime.

Methodology: The Euler equations are solved with ENS3DAE using a two-block half-million node H-H grid for a four-percent-thick rectangular wing of symmetric, parabolic-arc sectional geometry at zero angle of attack. The wing's control surface is a half-span, quarter-chord trailing-edge flap at one-degree deflection. A structurally elastic beam model composed of five modes represents the wing; modes are transferred to the aerodynamic grid using the infinite-plate spline. Static, aeroelastic solutions are computed with ENS3DAE for a variety of freestream dynamic pressures q through time integration and compared to solutions obtained with CAP-TSD, an algorithm for calculating the nonlinear, transonic small-disturbance equation. The ENS3DAE grid is somewhat finer than the CAP-TSD grid, but with an equivalent spanwise distribution of grid lines for validation. The ratio of aeroelastic roll moment to rigid roll moment is a measure of control surface effectiveness and serves as a basis of comparison for the two algorithms.

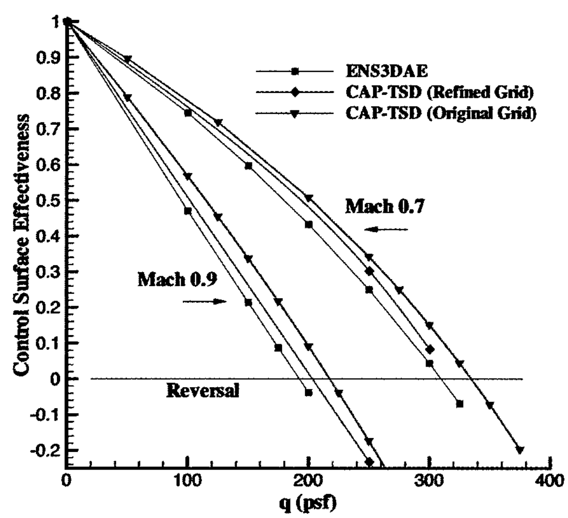
Results: Excellent agreement is obtained between ENS3DAE and CAP-TSD for control surface effectiveness as a function of dynamic pressure. The differential (bottom-top) pressure coefficient from ENS3DAE for the rigid wing at Mach 0.9, as represented by coloration of the surface grid, is shown at bottom left. The transonic lateral bleeding of the differential pressure coefficient inboard of the flap is particularly evident. At bottom right is the quantitative comparison of ENS3DAE and CAP-TSD at subsonic and transonic Mach numbers. The comparison is improved when the CAP-TSD grid is refined to near that of the ENS3DAE grid. Reversal is established at large values of q when flap deflection generates negative angles of attack at outboard stations and a net roll moment of sign opposite to that of the rigid case.

Significance: The ability to design and analyze flexible wings has been advanced by cross-validating algorithms based on the Euler equations and the transonic small-disturbance equations for control reversal. Validation of the nonlinear, yet very efficient, CAP-TSD algorithm suggests its use in the preliminary design of transonic wings. Validation of the higher fidelity ENS3DAE algorithm provides confidence in the application of this tool to aeroelastic problems that are not well suited to small-disturbance analysis.

JWCO: Precision Force



Differential coefficient of pressure for rigid wing at Mach 0.9



Comparison of control surface effectiveness

High Alpha Aerodynamics of the F-22 Fighter Aircraft

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HPC Computer Resource: Cray T90 [NAVO MSRC] and Cray J932 and Cray T916 [ARL MSRC]

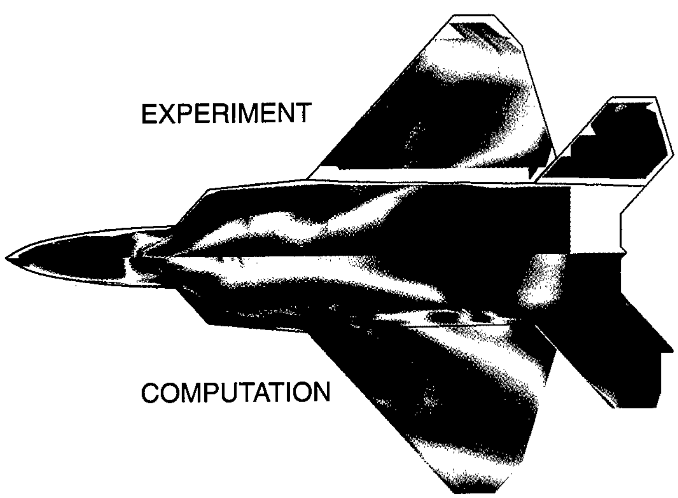
Research Objective: To combine advanced numerical techniques to analyze the external flow field of the F-22 fighter aircraft at high angles-of-attack. Accurate prediction of vortical flows for full aircraft configurations demands mature CFD technologies in the areas of turbulence modeling, grid generation, and numerical algorithms.

Methodology: The full Navier-Stokes equations are solved using the implicit Beam-Warming algorithm. The overset grid method is used to facilitate simple gridding across various components of the complex full aircraft configuration. The two-equation κ-ε turbulence model is chosen to provide a general model for the effects of turbulence in the flow field. The developed code FDL3DI has been optimized for operation on large-scale vector processors and may be easily adapted to operation on massively parallel platforms by exploiting the overset grid method.

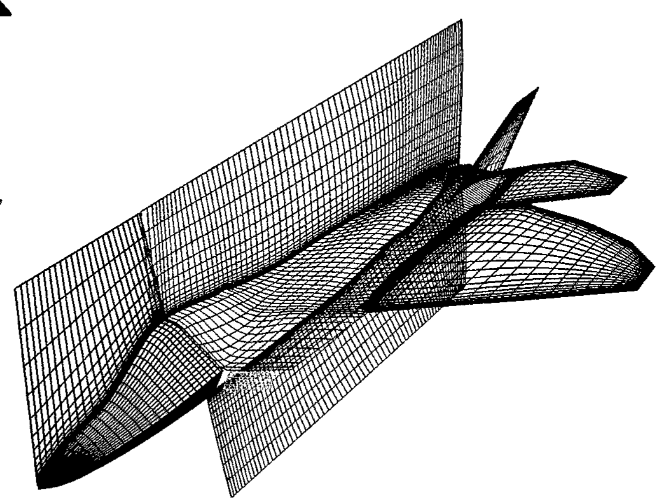
Results: Computations are made for conditions of subsonic Mach number at angles-of-attack of 10, 20, and 30 degrees. A computation has also been performed at 24 degrees angle of attack and 6 degrees yaw. Both experiment and computation show the low-pressure footprint of the strake vortex, its trajectory over the fuselage, and subsequent merging with the main wing vortex. The computation also predicts the compression regions in front of the canopy and the aft-fuselage observed in the experiment. Comparison of the surface pressure prediction with experiment is reasonable. The low-pressure footprint due to generation of vortices is predicted nicely.

Significance: The development work in this effort will enable us to have a reliable CFD tool to provide accurate flow predictions for such complex configurations. This tool enables analysis of design changes and modifications to full aircraft configurations at a reduced cost. Preliminary investigations of proposed new aircraft could also be performed in an efficient manner to impact the design cycle.

JWCO: Precision Force



Comparison of computation of surface pressure with experiment, Mach 0.4 at 20-degree angle of attack



Grid system for the F-22 aircraft

Interaction of a Leading-Edge Vortex with a Vertical Tail

D.P. Rizzetta
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HPC Computer Resource: Cray C90 [CEWES MSRC]

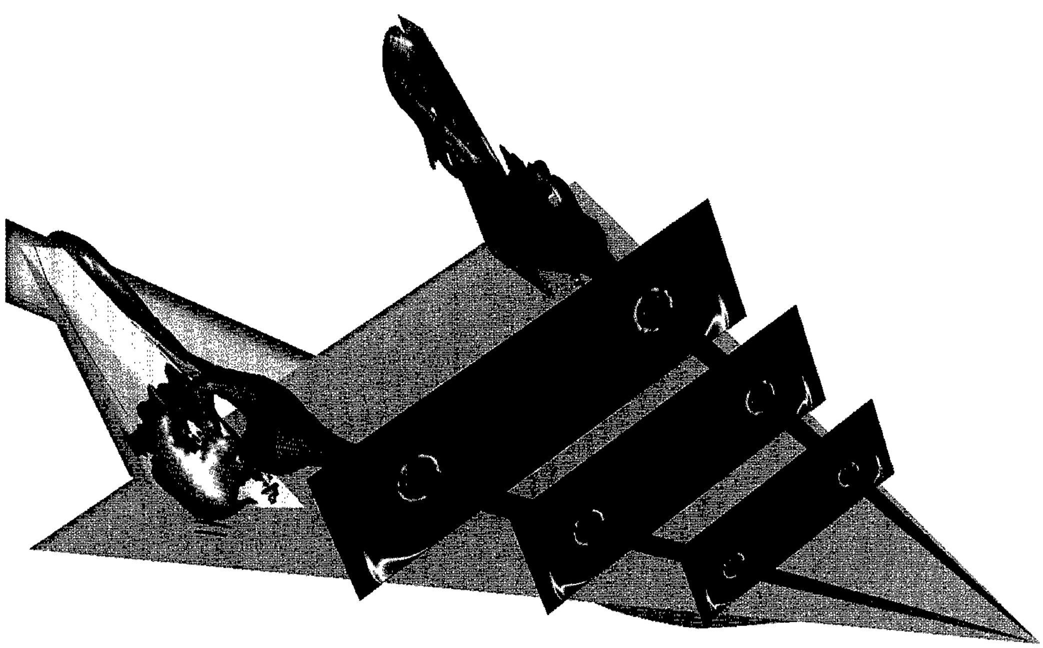
Research Objective: Streamwise vortices, which develop at the leading edge of wings in modern fighter aircraft, are used to augment lift and enhance performance and maneuvering capabilities. In the high angle-of-attack subsonic flight regime, these vortices may impinge on aerodynamic surfaces such as a fin or tail, and may result in efficiency loss, vibration, and adverse stability and control. Vortex breakdown can occur, causing tail buffet with a potential for fatigue-induced structural failure. The objective of this work is to investigate these situations numerically so that the adverse effect of vortex impingement may be mitigated or eliminated.

Methodology: The physical situation is modeled numerically by solving for the flow about a fighter configuration having a delta wing planform and twin vertical tails. Solutions are obtained to the unsteady three-dimensional compressible Euler and Navier-Stokes equations, and two different turbulence models are investigated. A fully vectorized, highly efficient computer code (FDL3DI) that uses an implicit approximately factored finite-difference algorithm is used for the computations, which are carried out on an overset zonal mesh system.

Results: The interaction between a leading-edge vortex and a vertical tail, which resulted in vortex breakdown, was successfully simulated by numerical computation. It was found that the Euler solution and one turbulent Navier-Stokes calculation reproduced observed features of the flowfield. Characteristics of the interaction were elucidated, and comparison was made with experimental data.

Significance: The ability to simulate vortex/tail interaction and to understand its basic features is the first step in controlling undesirable effects. This will allow for design improvement so that vortex-induced performance degradation and structural failure may be eliminated, thereby increasing efficiency and service life and decreasing maintenance costs.

JWCO: Precision Force, Joint Readiness and Logistics



Impingement of leading-edge vortices on surfaces of twin-tail fighter configuration

Numerical Fluid Dynamic Simulation of Parachute Clusters

J. Sahu
Army Research Laboratory, Aberdeen Proving Ground, MD
R. Benney
Natick Research, Development, and Engineering Center, Natick, MA
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Rockwell International Science Center, Thousand Oaks, CA

HPC Computer Resource: Cray C90 [CEWES MSRC] and SGI PCA [ARL MSRC]

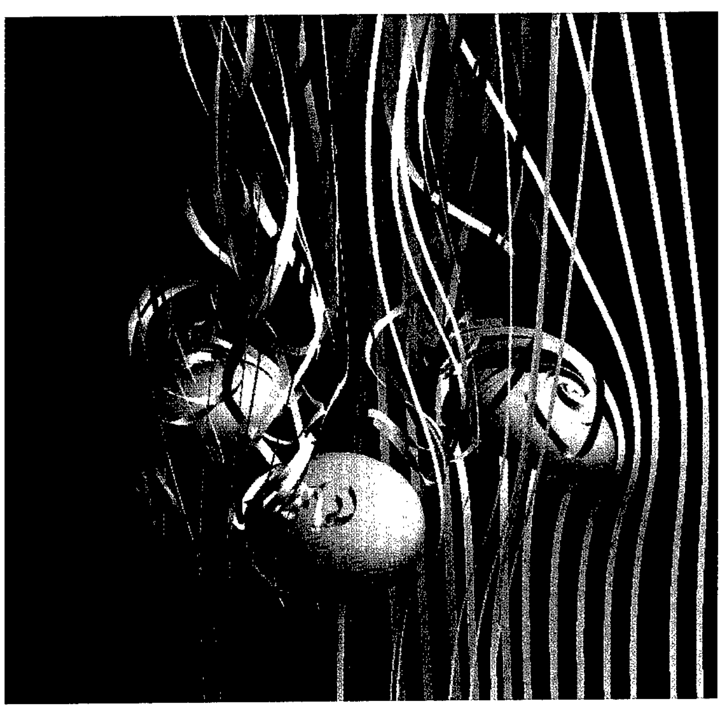
Research Objective: To develop a capability to compute the aerodynamics and terminal descent characteristics of parachute clusters associated with parachute deployment, flight, and guidance.

Methodology: Three-dimensional Navier-Stokes incompressible CFD codes are used to calculate the pressure and velocity fields around a cluster of round parachutes. Both structured and unstructured techniques have been evaluated for computational efficiency. Pressures over the inner and outer surfaces of the parachutes in the cluster are integrated to provide the net aerodynamic forces and moments acting on the canopies. A manual iterative process is used to determine the expected stable configuration for the cluster geometry by determining the condition at which the net forces and moments about the payload (origin) are zero.

Results: The results given here are the first predictions of aerodynamic flow field and descent characteristics for a cluster of three half-scale C-9 parachutes. The equilibrium angular location of the canopies predicted by the CFD computations is found to be in good agreement with available experimental data. These computational solutions provide, for the first time, an understanding of the flow field in and around parachute clusters.

Significance: This investigation has taken a major step in developing a computer tool that can be used to reduce the number of manufactured prototypes, as well as to reduce the need to perform multiple drop tests in different cluster configurations. This new capability has a great potential to assist in the development of improved parachute cluster design, which is essential to early entry and logistic resupply of forward projected forces.

JWCO: Military Operations in Urban Terrain



Particle traces show the flow pattern for a parachute cluster from bottom to top.

Aerodynamic Control of Theater Defense Missiles Using Jet Interaction

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D.R. McClure
THAAD Project Office, Huntsville, AL
A.L. Dang
ADRC, Inc., Huntsville, AL

HPC Computer Resource: Cray C90 [NAVO MSRC]

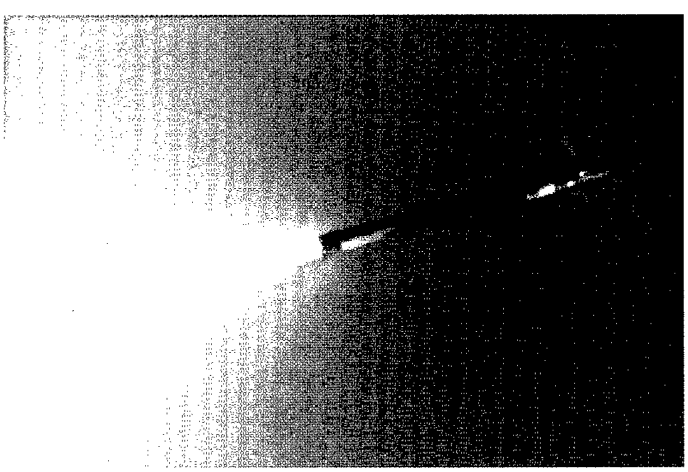
Research Objective: To provide a basic understanding of the different aspects of jet interaction (JI) control and to generate critical data so that an efficient and robust autopilot can be designed and tested for use across the entire THAAD battlespace.

Methodology: High-order upwind numerical algorithms are being used to solve the compressible Navier-Stokes equations for the THAAD interceptor using JI control. The hot jet exhaust is modeled as a single species with the equivalent thermodynamic properties of the chemically reacting liquid propellant. The key is to correctly capture the jet expansion and plume size so that the predicted aerodynamic interaction between the exhaust and the free stream flow over the missile provides a good estimate of the surface pressure as a function of Mach number, altitude, and angle of attack. The surface pressure is integrated to provide force and moment data for use in autopilot trade studies and wind tunnel data extrapolation.

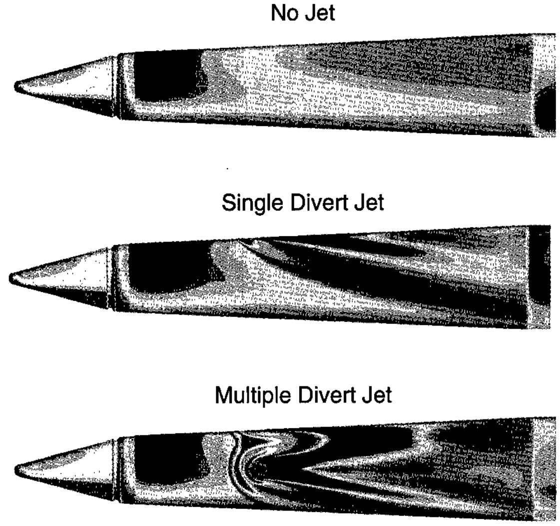
Results: Aerodynamic data are being generated to assist in the development of a scaling law that will predict full-scale, hot jet performance from subscale, cold jet tests. This is particularly important for multiple jet interactions in which the simple addition (superposition) of single jet results does not adequately predict multiple jet performance. The multiple jet exhaust creates a nonlinear interaction footprint on the surface of the kill vehicle that changes the original leverage created by the jet thrust. CFD results are also being used to expand the matrix of available aerodynamic data for autopilot design and to investigate the effect of the time delay between the divert thruster startup and the development of the aerodynamic interaction zone.

Significance: Ground testing of jet interaction phenomena is generally limited to cold jet exhaust and subscale models due to the limited size of existing wind tunnels and to the difficulties inherent in continuous flow testing of chemically reacting jet plumes. The present CFD capability allows cold gas tunnel data to be more effectively extrapolated to full-scale flight conditions with a hot jet. Modifications to existing cold gas JI models can now be implemented to account for hot gas effects that are not adequately simulated in ground tests.

JWCO: Joint Theater Missile Defense



Purging jet reaction controls prior to activation



Pressure contours during the firing of multiple divert jets on the THAAD interceptor

Titan IV Ignition Overpressure Analysis

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Lockheed Martin, Denver, CO

HPC Computer Resource: SGI Origin 2000 [ASC and ARL MSRCs]

Research Objective: To develop a detailed understanding of (1) the flow interaction between the solid rocket motor (SRMU) ignition and the nearby surrounding launch stand and environment, and the effects on the nozzle side load; and (2) the overall process of flow interaction with the full launch duct, including the shock wave that reflects back to the vehicle.

Methodology: The model used for this study is the three-dimensional hydrocode SHARC. This code is used because of its accurate shock modeling, coupled with complex geometry capabilities, and multi-gas capability. SHARC is an inviscid, compressible model with orthogonal grid. The grid for this case has 12 million cells. SHARC is fairly memory efficient and relatively quick running and robust, considering the size of the model. The overall physical size of the model, while still having the fine resolution to capture shock propagation accurately, has required the extremely large grid. This requires fairly large RAM along with extremely large disk space requirements and long run times.

Results: The full launch duct model has been run to 350 milliseconds, with good agreement to ground data pressure measurements. That case required 350 CPU hours and 800 megabytes of RAM. The ongoing case for the near-field effects on the nozzle load includes asymmetric initial conditions due to the plume from the gas hydraulic power unit (GHPU) that operates before SRMU ignition. The asymmetric pressure field, including internal flow separation, creates the nozzle load.

Significance: Detailed understanding of the ignition overpressure phenomena has progressed significantly with this modeling. This analysis provides details of the environment previously available only through very expensive hot-fire testing. For example, sensitivity studies of asymmetric GHPU exhaust on the nozzle load can be defined, and the velocity profiles in the launch duct can be determined. Furthermore, some gas properties such as density, temperature, and velocity can be visualized in the model, whereas in a test, these properties cannot be measured without intrusion and perturbation of the flow itself.

JWCO: Joint Readiness and Logistics

Snapshot of the pressure field around the launch duct at 290 ms after motor ignition. Both the initial waves, which progress axially up the vehicle, and the exit wave from the duct opening, which travels laterally back to the vehicle, are visible.

Turbulent Flow About High-Speed Naval Surface Combatants

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HPC Computer Resource: Cray C916 [NAVO MSRC]

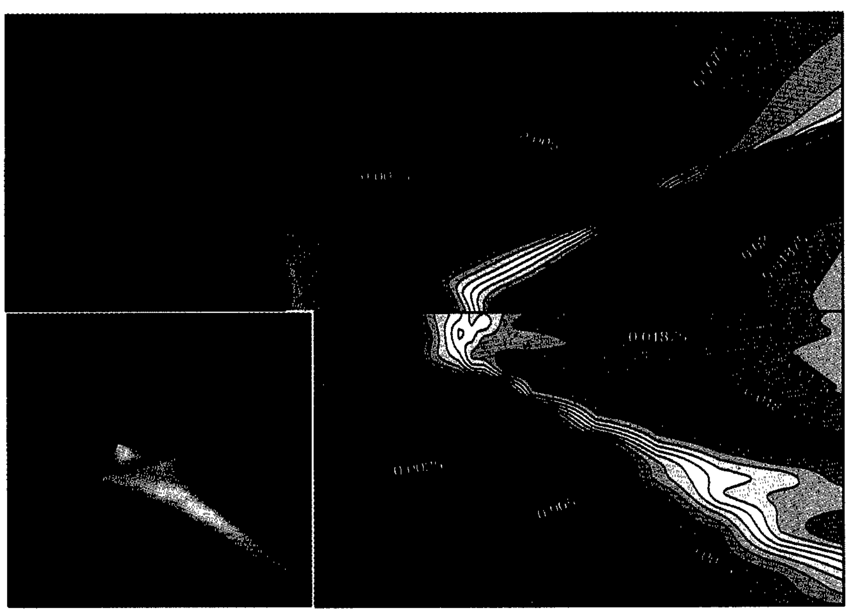
Research Objective: To extend to high-speed naval surface combatants the recent progress on the inclusion of viscous (frictional) effects in computational analysis and prediction of free-surface flows about ships. To increase the understanding of transom stern flows and thereby facilitate the improvement of transom stern design.

Methodology: The DTNS3D Reynolds-averaged Navier-Stokes computer code was previously extended to include nonlinear free-surface boundary conditions and validated for hulls with cruiser sterns. The current work extends its application to the more challenging transom stern geometry characteristic of high-speed naval surface combatants. Hulls with transom sterns, such as typical rowboats, terminate abruptly with a large, essentially flat, surface area at the stern. At high speed, the flow separates from the hull at the lower edge of the transom and the hull boundary-layer wake is adjacent to the water surface. The gridding strategy maintains the boundary resolution into the wake to capture this strong viscous/free-surface interaction.

Results: Computational predictions have been obtained for the steady free-surface flow about model 5415, a scale model of the DDG-51 Aegis destroyer, the Navy's newest surface combatant. The computed stern region wave heights are compared in the figure with measured data from recent towing tank tests of the model. Although there are differences, mostly due to unsteady wave breaking in the model test, the agreement is striking, especially with respect to height, shape, and location of the prominent plateau just downstream from the stern. Comparisons of the computed results with results from the widely used inviscid methods have also been carried out. It was shown that wave heights predicted for the inviscid flow are close to those predicted for the viscous flow except in the stern region where viscous effects are significant.

Significance: Capturing the viscous/free-surface interaction of the hull boundary layer wake with the water surface now allows accurate prediction of transom stern wave patterns. The developed tools will facilitate the improvement of transom stern design for improved ship performance and aid in the evaluation of innovative configurations such as sterns designed for water jet propulsion. Performance improvements and the ability to achieve them with reduced design time will provide significant cost savings.

JWCO: Information Superiority, Combat Identification



Aerial view of computed (top half) and measured (bottom half) stern waves generated by model 5415. The model is moving to the left and the stern is shown in black. Wave heights are in units of model length. Inset: Perspective view of computed waves.

External Store Captive Carriage Forces and Moments

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HPC Computer Resource: SGI PCA [NAWCAD DC]

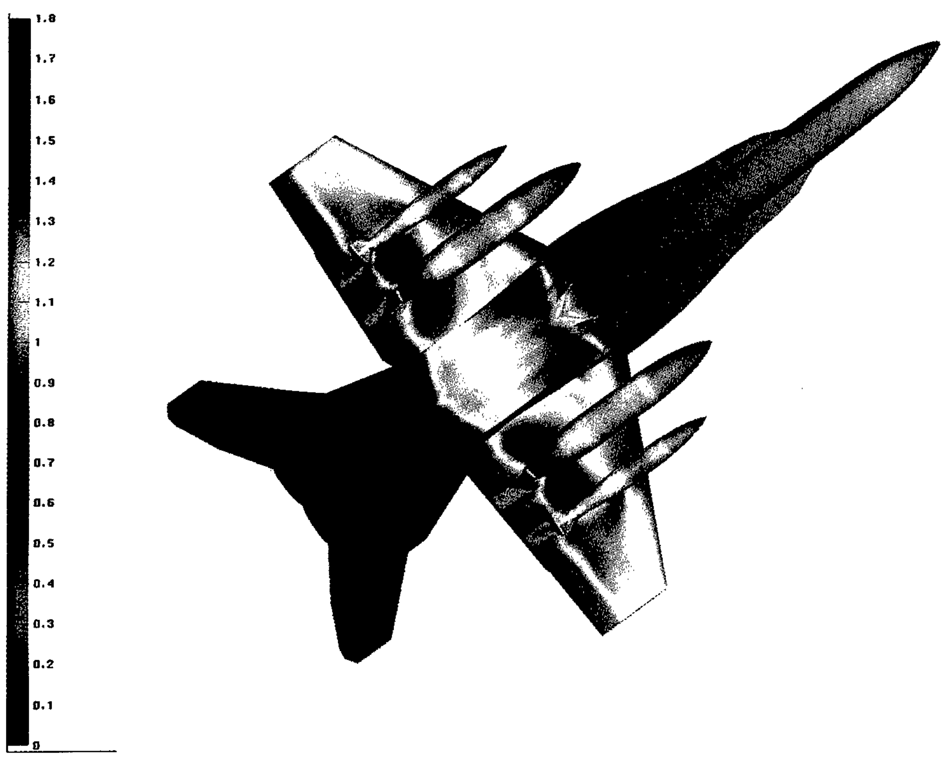
Research Objective: To evaluate a CFD code's ability to accurately compute the forces and moments of externally mounted stores on Navy fighter aircraft.

Methodology: The unstructured Cartesian Euler/Navier-Stokes flow solver SPLITFLOW was used to calculate the forces and moments of the JDAM munition mounted on the outboard pylon of an F/A-18C aircraft in the transonic and low supersonic flight regime. The calculations were performed in the inviscid Euler mode utilizing approximately 800,000 cells. The code is solution adaptive based on user-specified flow gradients that were chosen to be Mach number and pressure.

Results: The code accurately predicted a doubling of the yawing moment acting on the store over a speed range from 0.9 to 0.925 Mach. Accurate captive carriage forces and moments are required to determine jettison and launch trajectories.

Significance: To clear a weapon for use in the Fleet, every combination of airspeed, load factor, roll rate, and angle of attack must be considered to safely release the weapon from the aircraft. To date, the only accurate means of obtaining the aerodynamic forces and moments that determine the weapon's trajectory is by extensive and costly (about $4,000/hour) wind tunnel and even more expensive flight testing. The use of validated CFD codes for calculating forces and moments as well as distributed pressure loading and off-body flow visualization has the promise of cutting the required wind tunnel testing time in half for new weapon clearance, thereby greatly reducing cost for providing enhanced capability to the Fleet.

JWCO: Precision Force



Inviscid Mach number contours on the lower surface of an F/A-18C with 330-gallon tank on the inboard pylon and the JDAM on the outboard pylon at Mach 0.9 and $\alpha = 0$

CFD Modeling of BAT Submunition Dispersal

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Army Research Laboratory, Aberdeen Proving Ground, MD

HPC Computer Resource: Cray C90 [ASC MSRC] and SGI PCA [ARL MSRC]

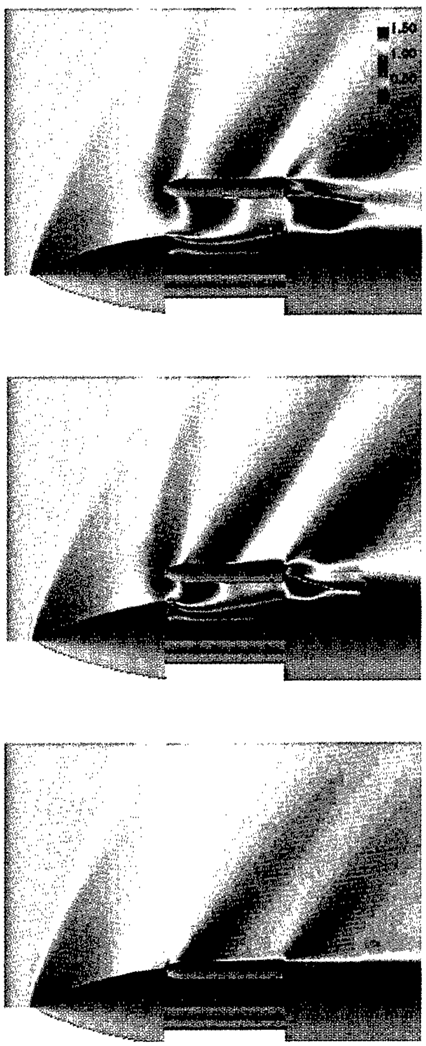
Research Objective: To develop a capability to compute the aerodynamics of complex multibody projectile and missile configurations and bodies in relative motion.

Methodology: This research involves the application of the versatile Chimera numerical technique to both steady and time-dependent multibody configurations. This multidisciplinary work couples the solution of the Navier-Stokes equations with the solution of the six degree-of-freedom equations of motion. The complexity and the uniqueness of the problem result from the multiple bodies being in relative motion to each other, thus requiring a time-dependent solution. The Chimera technique, which is ideally suited to this problem, involves generating independent grids about each body and then oversetting them onto a base grid to form the complete model. With this composite overset grid approach, it is possible to determine the unsteady aerodynamics associated with the bodies in relative motion without the need to re-grid.

Results: CFD modeling has provided physical insight into the complex unsteady aerodynamic interference flow field and design information to ensure successful dispersal of the brilliant antiarmor (BAT) submunitions from a tactical missile system (TACMS). Computed results show the details of the three-dimensional aerodynamic interference flow field, which includes both the missile-to-BAT as well as BAT-to-BAT interactions.

Significance: This work represents a major increase in capability for determining the aerodynamics of multibody projectile and missile configurations and has been successfully applied to the Army TACMS BAT program. The developed technique improves the Army's technical capability in the accurate and realistic numerical prediction of interference effects and aerodynamics that is required for the improved design and modification to current and future multibody missile and projectile configurations.

JWCO: Precision Force, Joint Theater Missile Defense



Mach contours showing the interference flow field between the missile and the BAT submunition at different radial locations

The Design of ODOBi, a Partially Confined Detonation Facility

C.A. Lind, J.P. Boris, C.R. Kaplan, T.R. Young, Jr., and E.S. Oran
Naval Research Laboratory, Washington, DC

HPC Computer Resource: SGI PCA [NAVO MSRC]

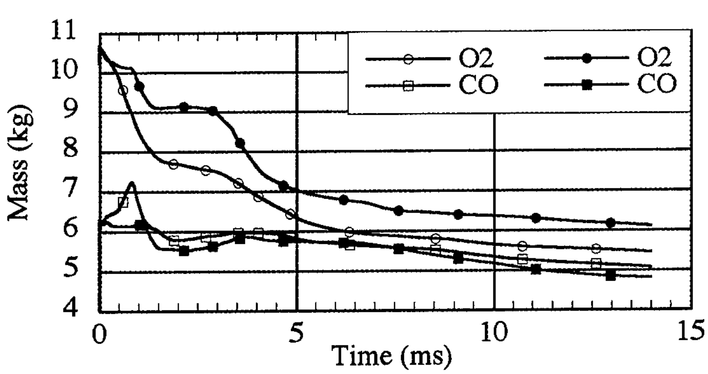
Research Objective: To perform time-dependent simulations of the elimination, by detonation, of unexploded ordnance, unwanted propellants, and demilitarized munitions within the ODOBi, a geometrically complex, partially confined detonation facility. These simulations will be used to develop a procedure for eliminating these materials in the most environmentally sound and cost-efficient manner.

Methodology: FAST3D is a general-purpose, scalable CFD model based on the high-resolution flux-corrected transport (FCT) algorithm for solving generalized continuity equations. The FAST3D model combines the FCT algorithm with the virtual cell embedding (VCE) technique for efficient treatment of the subgrid scale features of geometrically complex domains. FAST3D has been implemented on new, cost-effective, parallel computer architectures.

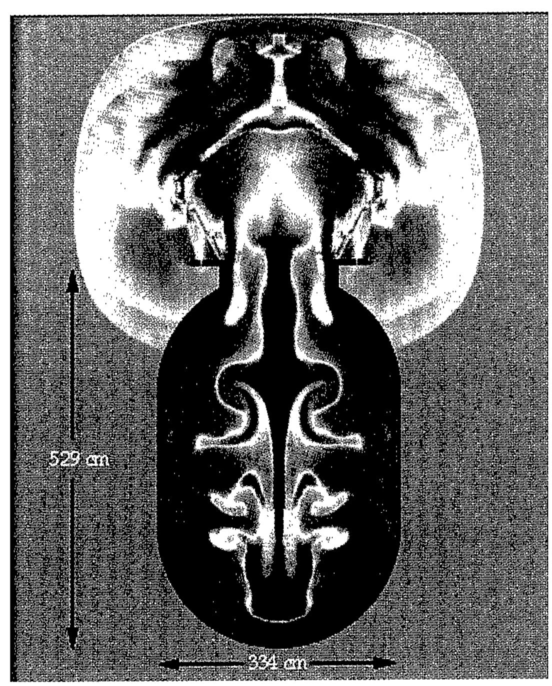
Results: Simulations were performed of several design options for the ODOBi facility, now in operation at Dugway Proving Ground, Utah. These simulations identified a number of problems, including high pressures that could damage the chamber and excessive noise in the environment. Parameters in the simulation included the position, size, and shape of the initial explosion, the effects of chemical reactions, and the shape of the containment facility.

Significance: Safe and cost-effective elimination of the more than 500,000 tons of obsolete explosives is a major DoD objective and a necessary prerequisite for base reductions and re-use of land resources. The computer simulations are being used to design a geometrically complex, partially confined detonation facility. This partially confined approach promises to allow the disposal of unexploded ordnance and surplus energetic materials in an environmentally safe manner. This approach is equally promising for destruction of biological and chemical weapon materials.

JWCO: Military Operations in Urban Terrain, Chemical/Biological Warfare Defense and Protection



Comparison of the integrated species masses within the ODOBi for the detonation of a uniformly shaped charge (red lines) and a nonuniformly shaped charge (blue lines)



Temperature contours 8 ms after detonating a 50-lb uniformly shaped RDX charge at a height of 1.82 m

Improved Combustion Control with Coaxial Jets Systems

F.F. Grinstein
Naval Research Laboratory, Washington, DC

HPC Computer Resource: Cray C90 [CEWES MSRC]

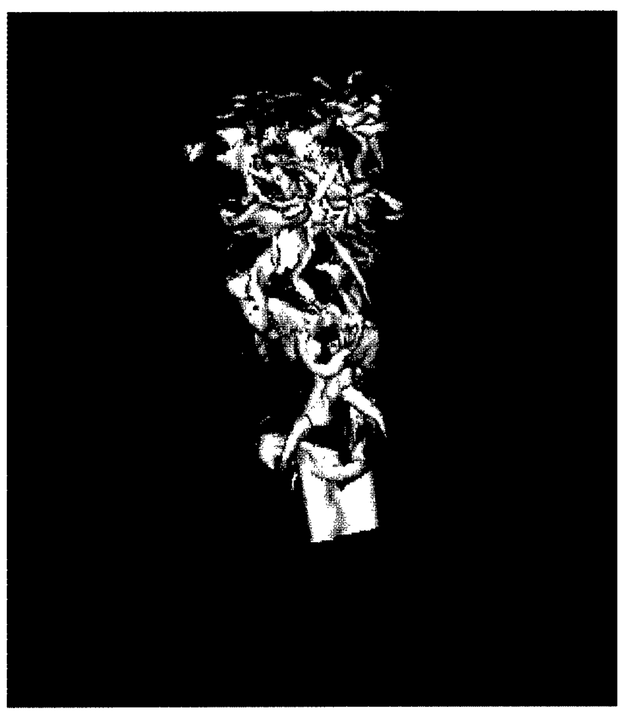
Research Objective: To achieve efficient and clean combustion in propulsion engines involving jet flames. The entrainment-enhancing performance of countercurrent jets is the focus of the research efforts, seeking understanding of how it is affected by initial conditions and chemical exothermicity, examining whether it can be improved by using low-aspect-ratio rectangular nozzles, and addressing how it is affected by confinement in simple dump ramjet combustor configurations.

Methodology: We performed time-dependent three-dimensional (3-D) computer simulations of coaxial countercurrent rectangular jets involving entrainment actuation at the jet exit by means of a secondary reverse (suction) flow enforced around the primary jet perimeter. The 3-D reactive-jet numerical model solves the time-dependent, compressible conservation equations for mass, momentum, and energy for ideal gases using flux-corrected transport (FCT) algorithm timestep-splitting techniques on structured grids, and appropriate inflow/outflow open-boundary conditions. The multispecies diffusive transport and finite-rate chemical reaction processes are coupled with convection using timestep-splitting techniques.

Results: Detailed comparisons were set up between free and countercurrent jet performances in regimes of practical interest, and the effects of changing initial conditions of the primary jet were also assessed. Flow visualizations of the developed jet regimes indicate dominant flapping and helical modes, and enhanced entrainment associated with the co-annular suction. The characteristic underlying vortex dynamics of these jet systems was documented for the first time.

Significance: This research examines ways of increasing the range and speed of missiles and other Navy aircraft by enhancing the performance of combustors used in the propulsion systems. The investigations address the impact of improved jet combustion control strategies that combine active and passive entrainment enhancing concepts by using countercurrent rectangular jets. The understanding gained with this research aids in the development of compact combustors that have diminished fuel consumption and increased power output.

JWCO: Joint Readiness and Logistics



Instantaneous flow visualization of a countercurrent square jet, based on distributions of the mixing fraction (color) superimposed on isosurfaces of the vorticity magnitude (gray). The flow direction is from bottom to top. The initial conditions at the jet exit plane are depicted at the bottom (blue: primary jet; red: co-annular suction; green: reflecting wall).

Analysis of Chemical Oxygen-Iodine Laser (COIL) Optical Quality

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Air Force Research Laboratory, Kirtland AFB, NM

HPC Computer Resource: Cray C90 [CEWES and NAVO MRSCs] and IBM SP [MHPCC DC]

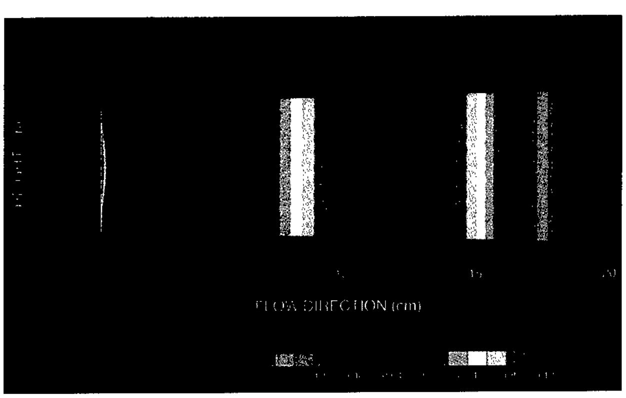
Research Objective: To investigate chemical oxygen-iodine laser (COIL) device flows in the plenum, nozzle, and laser cavity regions to evaluate power capabilities, flow requirements, cavity optical quality, and pumping capacities by including effects of sidewall injection and mixing, chemical reactions, and optical power extraction.

Methodology: Analyses were done on a COIL laser cavity to quantify the flow disturbances and to translate those disturbances into a value for optical quality. An implicit, nonlinear, chemically reacting, time-dependent Navier-Stokes solver that incorporates laser power extraction was used. To make the analyses tractable, the problem was broken into two contributions to cavity optical quality that are later combined to obtain the total value. The small-scale portion contains microscale disturbances whose source is the transverse iodine injector flow mixing with the primary flow. The large-scale portion contains macroscale disturbances originating from nozzle blades, sidewalls, and cavity shrouds.

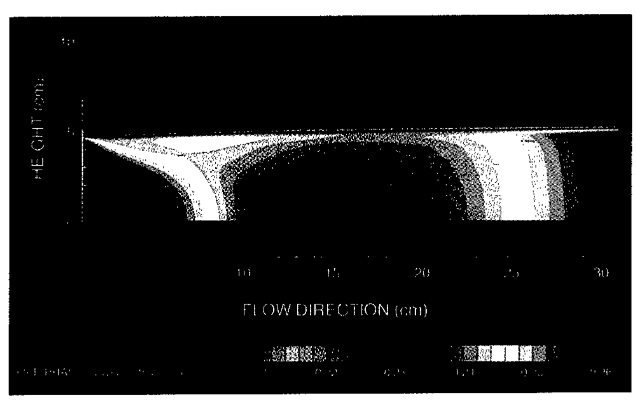
Results: Results for both the small-scale and large-scale calculations are found in terms of the single-pass wavefront error, called the optical path difference (OPD). This is a measure of the amount of distortion, expressed as the number of interferogram fringe shifts, applied to a laser beam passing through or emanating from a laser device. The greater the OPD field magnitude and the larger the OPD field gradients, the less energy will be propagated to the target. These results show that the microscale OPD effects are 1-D in nature, varying primarily in the laser gas flow direction, and of low spatial order, meaning that they are relatively easy to correct. The COIL medium quality is shown to be dominated by macroscale effects, primarily pressure waves generated from the interactions between the flow and boundary layer on the cavity shrouds.

Significance: The capability to analyze COIL medium quality in detail is of significant benefit in the design and evaluation of COIL devices to perform the tactical and strategic defense missions being contemplated for high-energy laser systems. The device medium quality is the first in a chain of elements that must be combined to determine the laser beam quality as the laser exits the beam director. This beam quality, when combined with the effects of atmospheric disturbances encountered during propagation to the target, will determine the effectiveness of the beam at the target.

JWCO: Joint Theater Missile Defense



Microscale OPD map with tilt removed (flow from left to right)



Macroscale OPD map with tilt removed (flow from left to right)

Missile Exhaust Plume Phenomenology

H.B. Ebrahimi
Sverdrup Technology, Inc., Arnold Engineering Development Center, Arnold AFB, TN
W.H. Calhoon, Jr.
SPARTA, Inc., Air Force Research Laboratory, Edwards AFB, CA

HPC Computer Resource: Convex SPP-2000 [AEDC DC] and SGI PCA [ARL and NAVO MSRCs, and TARDEC DC]

Research Objective: To determine the effect of three-dimensional (3-D) features, real engine characteristics, and missile-plume interactions on rocket exhaust radiation signatures.

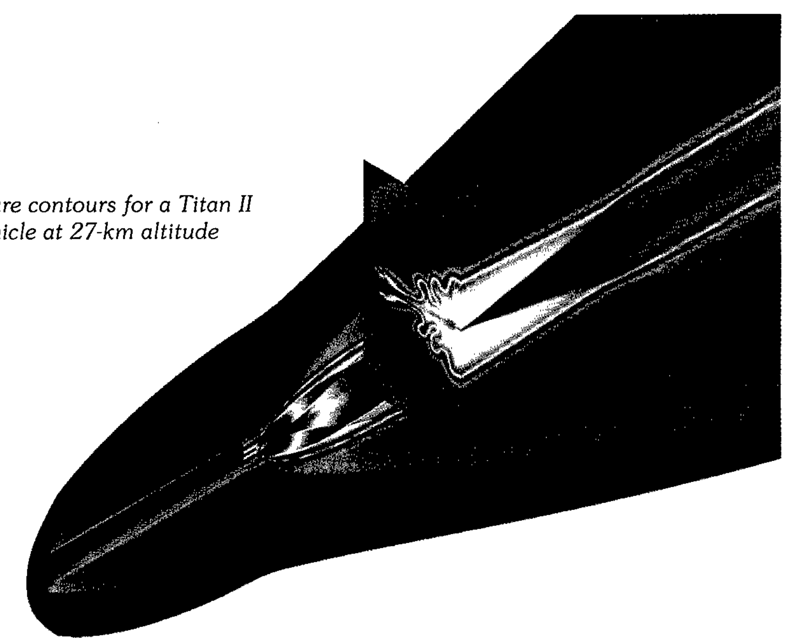
Methodology: Missile body and plume flow fields are analyzed using a structured compressible Navier-Stokes flow solver implemented with multi-zone capability to allow complex multiple engine missile systems to be simulated. Computational efficiency is achieved through optimized shared-memory parallelization of the flow solver and also through the use of a parabolized form of the Navier-Stokes equations in hyperbolic regions of the flow.

Results: Coupled engine-nozzle-missile-plume simulations were obtained for the Titan II missile at two altitudes, and for other missiles at a range of operating conditions. These simulations have demonstrated for the first time: the dependence of plume signature on the roll angle of multiengine missiles; the impact of engine oxidizer/fuel striations and gas generator exhaust on radiation intensity; and the effect of 3-D flow on afterburning and, hence, on the spatial distribution of plume infrared radiation. In all cases, the computer simulations have been compared to flight or ground test data. In general, excellent agreement was obtained—not only in radiation levels, but also in the ability to reproduce experimentally observed spatial features.

Significance: The ability to accurately simulate the 3-D characteristics of rocket engine exhaust plumes over a wide altitude range will significantly improve our ability to reliably perform missile launch detection, tracking through burnout, and missile typing (to facilitate the post boost target discrimination function). It is also critical for accurately performing the aim point selection function in boost phase intercept (hit-to-kill) scenarios. Validated simulation models are also used to aid in the selection of sensor band passes and dynamic range parameters as well as to generate signature characterizations for missiles.

JWCO: Information Superiority, Precision Force, Joint Theater Missile Defense

Temperature contours for a Titan II launch vehicle at 27-km altitude



Hybrid Algorithm Development for Nonequilibrium Mixed Flows

C.K. Oh and E.S. Oran
Naval Research Laboratory, Washington, DC

HPC Computer Resource: TMC CM-500E [NRL DC] and TMC CM-5 [AHPCRC DC]

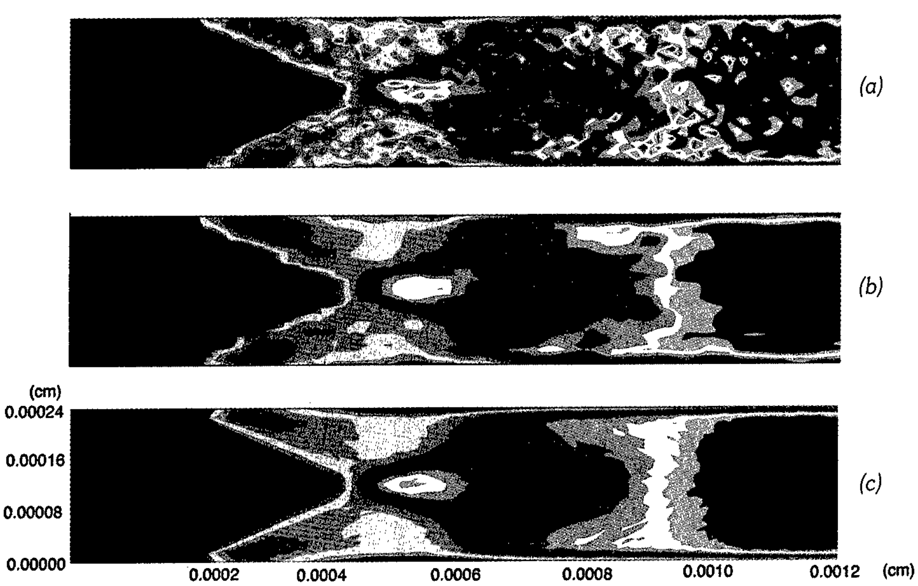
Research Objective: To develop an efficient, parallel hybrid algorithm for simulating flows in the mixed flow regime, in which the continuum approximation for fluid breaks down in some part of the flow system and the particle behavior has fundamental importance. Navier-Stokes (NS) and the direct simulation Monte Carlo (DSMC) - monotonic Lagrangian grid (MLG) methods are coupled to reduce the cost of DSMC computation using NS solutions while still capturing the mixed flow physics.

Methodology: DSMC is a statistically based particle method, and MLG is the method of handling complex particle data structures. Combining these two approaches provides a method that has automatic grid refinement for DSMC computations. This DSMC-MLG is coupled with NS, which is a continuum fluid approximation, to compute the mixed regime flows. In developing the hybrid algorithm, an interpolation from DSMC-MLG unstructured grid to NS structured grid is required. A bilinear grid interpolation technique was developed and successfully applied. Also, the NS code was modified to accept DSMC-computed variables such as transport coefficients and wall boundary condition. In this approach, DSMC provides the physically correct boundary conditions and transport coefficients in high-Kundsen-number flow regimes for the NS computation, and NS is then used to accelerate the DSMC solution to a statistically converged solution.

Results: DSMC-MLG and the NS methods have been successfully coupled on the Connection Machine. In this hybrid approach, NS computation is used to filter statistical noise from DSMC computation. Therefore, long time periods in which statistics must be collected to achieve a good DSMC solution are eliminated by a short pass through the NS computations.

Significance: The new computational capabilities developed in this study can be applied to many important physical systems in which laboratory experiments are difficult because of the broad range of time and length scales. Those systems include micro-electro-mechanical systems (MEMS), material processing devices, low-density chemical vapor depositions, plasma etch reactors, and micro-unmanned aerial vehicles (micro-UAV). All of these applications are areas of Navy and DoD interest.

JWCO: Joint Readiness and Logistics



Pressure contours of Mach 5 flow into a microchannel: (a) DSMC noisy steady-state solution, (b) NS filtered solution, and (c) DSMC converged solution. The NS filtered solution (b) shows very similar flow structure to DSMC converged solution (c). The computational times taken from (a) to (b) and from (a) to (c) are 6 seconds and 2.5 hours, respectively.

Adaptive Refinement and Structured Grids for Unsteady Aerodynamics

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Army Aeroflightdynamics Directorate, Moffett Field, CA

HPC Computer Resource: Cray C90 [CEWES MSRC]

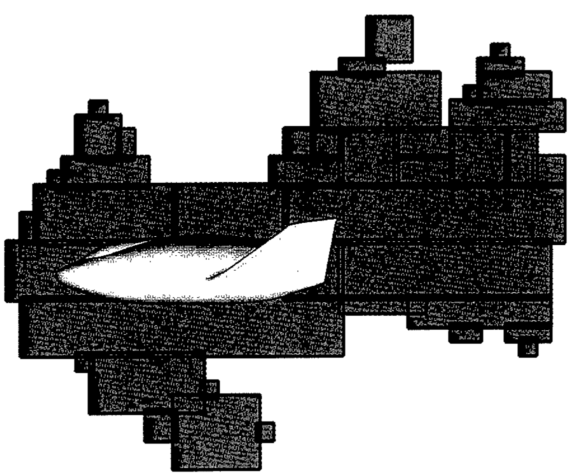
Research Objective: To develop robust adaptive refinement methods for unsteady geometrically complex (moving body) applications that exploit the computational advantages inherent in structured data.

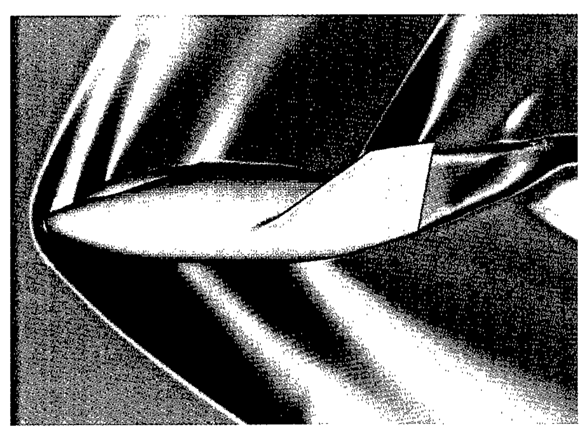
Methodology: The physical domain of complex problems is decomposed into near-body and off-body regions. The near-body domain is discretized with Chimera overset grids that need extend only a short distance into the field. The off-body domain is discretized with overset structured Cartesian grids (uniform) of varying levels of refinement. The near-body grids resolve viscous boundary layers and other flow features expected to develop near-body surfaces. Off-body grids automatically adapt to the proximity of near-body components and evolving flow features. The adaption scheme automatically maintains solution accuracy at the resolution capacity of the near-body system of grids. The approach is computationally efficient and has high potential for scalability. Grid components are automatically organized into groups of equal size, facilitating parallel scale-up on the number of groups requested. The method has been implemented in the OVERFLOW-D2 code being developed within CFD CHSSI projects.

Results: The adaptive refinement capability within OVERFLOW-D2 has been demonstrated on the X-38 crew return vehicle in a Mach 1.5 freestream, at 15 degrees angle-of-attack, and for a Reynolds number of 25 million.

Significance: Demonstration of OVERFLOW-D2 on a large-scale application such as the X-38 crew return vehicle is significant because of the broad class of problems of interest to the DoD that require the accuracy available through adaption and the computational efficiency realizable through structured data. Target problems of the method include unsteady moving geometry applications such as aircraft store separation, helicopter rotor-body interaction, crew escape systems, flight maneuvers, and launch vehicle staging.

JWCO: Precision Force





Boundaries of finest off-body grids (left) and Mach field after one adapt cycle (right)

Combustion of High-Energy Fuels

E.J. Chang and K. Kailasanath
Naval Research Laboratory, Washington, DC

HPC Computer Resource: Cray C90 [CEWES MSRC]

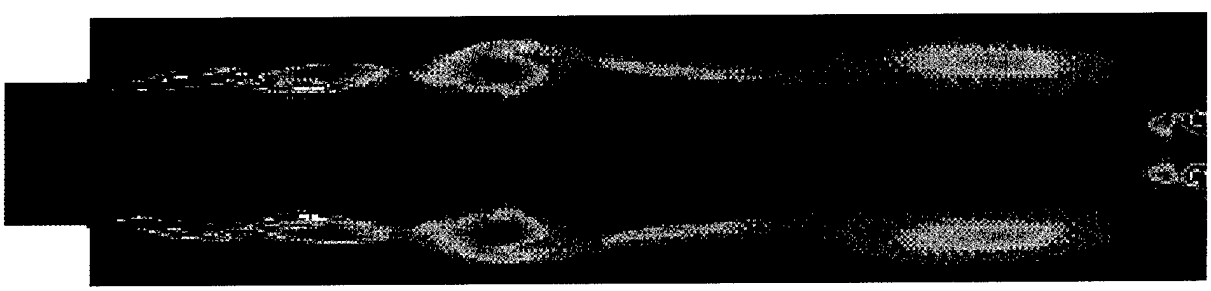
Research Objective: To develop a computational model of the combustion of high-energy fuels and to use the model as a tool to improve our understanding of the combustion of high-energy fuels. Understanding the combustion of high-energy fuels could lead to a major breakthrough in the quest to attain increased range and speed for missiles and other Navy propulsion systems.

Methodology: The unsteady gas phase flow in a ramjet combustor is computed by solving the conservation equations for mass, momentum, and energy using the flux-corrected transport algorithm. The fuel droplets' position in the flow field is determined by solving the Lagrangian equations of motion for the droplets, taking into account the inertial drag force that depends on droplet size and density. The fuel droplets are considered to be multicomponent, consisting of a solid cubane core surrounded by a liquid phase carrier. Evaporation of the droplets based on the local temperature and the rapid energy release during the microexplosion of these high-energy fuel droplets have been considered.

Results: The dynamics and microexplosion of high-energy fuels injected into an axisymmetric ramjet combustor have been numerically simulated. Parametric studies have been carried out to investigate the role of factors such as droplet size, fuel injection-timing, and acoustic forcing. In general, it has been observed that dispersion increases as droplets vaporize and that microexplosions can cause local flow disruption and even modification of the flow instabilities. In addition, by suitably choosing the size of the fuel droplet for a given flow velocity, attenuation or amplification of pressure fluctuations can also be achieved. This last observation has been used to demonstrate an interesting application for these high-energy fuels: as a secondary fuel-injection source to suppress combustion instabilities in ramjets.

Significance: Simulations such as those described here can have a major impact in the development and application of these high-energy fuels for DoD propulsion systems. Use of these fuels will provide a significant increase in the range and speed of missiles, leading to greater stand-off distances and lower casualties for our armed forces. Such simulations support reduced acquisition costs and reduced test and evaluation schedules for new systems. The new computational capability can also be used to investigate a variety of other DoD problems involving multiphase flow and combustion.

JWCO: Joint Theater Missile Defense, Joint Readiness and Logistics



The location of microexploding fuel droplets of 35-mm initial diameter is shown along with the vorticity distribution (blue: lowest; red: highest) in an axisymmetric ramjet combustor.

Numerical Simulation of Blast Wave Diffraction About Structures

J.D. Baum and H. Luo
SAIC, McLean, VA
R. Löhrner
George Mason University, Fairfax, VA

HPC Computer Resource: Cray C90 [CEWES MSRC]

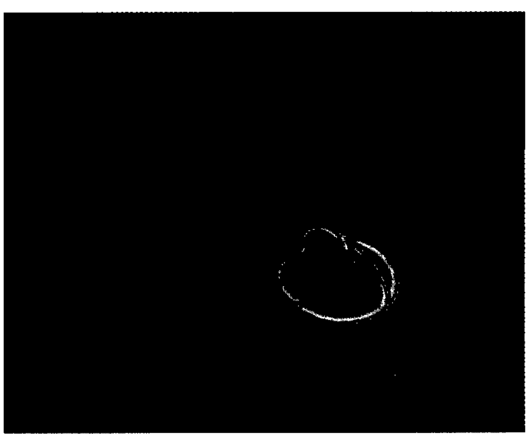
Research Objective: To develop a fully integrated computational fluid dynamics (CFD) and computational structural dynamics (CSD) methodology for the time-dependent simulation of blast wave interaction with structures. The developed methodology will model the complete detonation initiation and propagation, blast wave diffraction, and structural response phenomena, starting from the detonation of conventional or nuclear weapons, blast wave propagation in the free field, blast diffraction about the structures, blast loading on the structures, the resulting structural response, wave modification due to structural response, and blast propagation through the responding structure.

Methodology: Fully integrated state-of-the-art CFD and CSD algorithms are combined. The CFD methodology FEFLO97 is a recently developed three-dimensional, adaptive, finite-element, edge-based, arbitrary Lagrangian/Eulerian shock-capturing methodology based on unstructured tetrahedral grids. It is used for solving Euler and Reynolds-averaged turbulent, Navier-Stokes equations. FEM-FCT is a high-resolution, monotonicity-preserving algorithm. The CSD methodology DYNA3D uses unstructured grids and a spatial discretization that involves finite-element techniques, large deformation formulation for the solids, explicit time integration, and several material models, kinematic options, and equations of state.

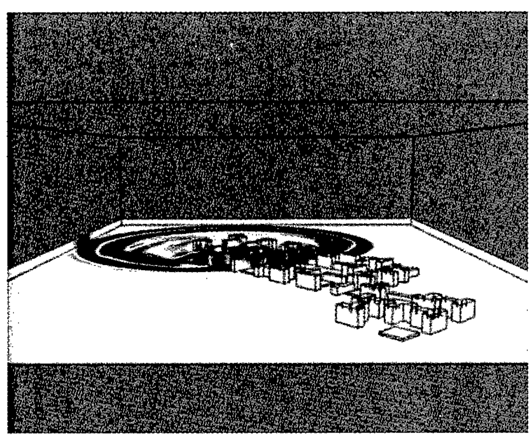
Results: The developed methodology has been applied successfully to both military and civilian applications. The results shown here model the terrorist attack against the U.S. Air Force base at Khobar Towers, Dhahran, Saudi-Arabia. The simulation modeled the detonation wave initiation, wave propagation, and diffraction around the many buildings of the compound to a distance of more than a kilometer. Results of the simulations compared fairly well with post-attack observations.

Significance: The coupled methodology enables a priori prediction of blast damage to underground command and control centers and other targets of military significance, thereby increasing targeting efficiency. Simultaneously, the methodology enables the cost-effective hardening of civilian and military facilities against terrorist attacks. Here, the numerical methodology was used as a forensic tool, to help pinpoint the size of the explosive charge.

JWCO: Military Operations in Urban Terrain



Pressure contours at an early time. Shock wave has just diffracted around the closest building.



Pressure contours at a later time. Notice the diffused shock wave within the village due to shock diffraction around the many structures.

Contaminant Transport Modeling for Consequence Management

J.P. Boris, T.R. Young, Jr., A.M. Landsberg, and B.Z. Cybyk
Naval Research Laboratory, Washington, DC

HPC Computer Resource: SGI PCA [NAVO MSRC]

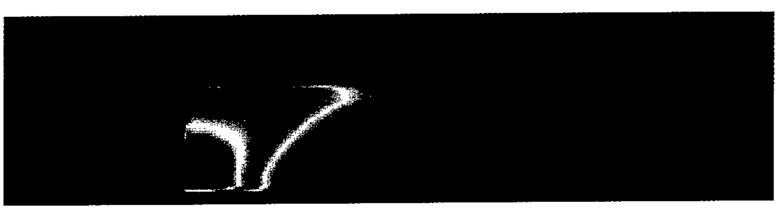
Research Objective: To further develop and mature a portable, complex geometry, contaminant transport model aimed at supporting consequence management operations for chemical/biological warfare.

Methodology: The CFD code FAST3D-CT solves the dynamic transport equations for air and airborne contaminants. Multispecies particle and gas phase contaminants can be initialized, sprayed, or injected from localized sources, transported, and diagnosed without restarting the model. A sophisticated turbulence model ensures that the flow correctly adapts to complex terrain with vertical and re-entrant surfaces and automatically generates local turbulence in passing through openings and over obstacles. The current version requires topographical and meteorological input data, although a detailed initial wind field can also be calculated internally.

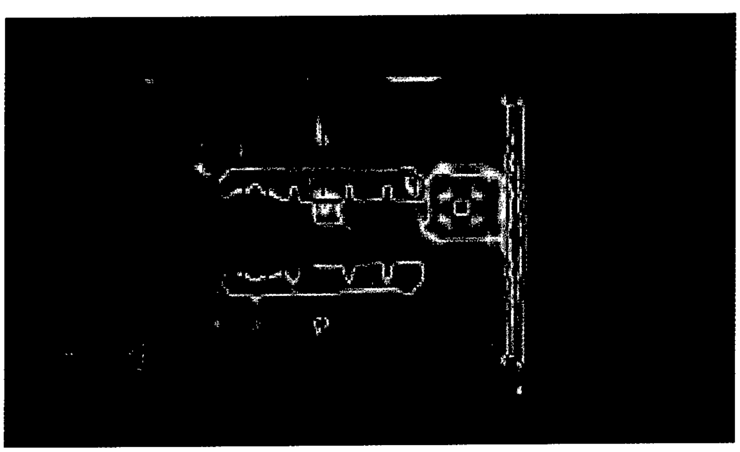
Results: Detailed simulations of *Bacillus gobigii* (BG)/propylene release trials were performed during an advanced concept technology demonstration (ACTD). Complete simulations of a convention center mock-up were performed on-line, in some situations in near real-time, using internal building measurements, HVAC conditions, and external meteorological conditions at the time and location of the trials. The full geometry was represented, including time-varying wind flows on the building exterior and a realistic rendition of the HVAC-driven flows inside the building. Based on these simulations, preliminary rules of thumb were developed to support the consequence management operations. Participation in this ACTD was sponsored by OSD Counter Proliferation and Chemical/Biological Programs.

Significance: The DoD is currently seeking to improve its modeling and simulation capability to help counter the threat posed by the worldwide proliferation of chemical and biological weapons. Detailed contaminant transport modeling that includes the effects of realistic complex geometry is central to any technology aimed at providing a timely, effective response to a chemical or biological threat or to assess the effects of an obscurant cloud. Real-time simulation of chemical/biological attack scenarios is potentially as valuable to the civilian community as to the DoD.

JWCO: Chemical/Biological Warfare Defense and Protection



BG deposited along the building floor and outside the door one hour after contaminant release



BG suspended in building (vertical cross-section) one hour after contaminant release

Effective Parallelization of an Implicit CFD Code

D.M. Pressel, K.R. Heavey, J. Sahu, J.P. Collins, and C.J. Nietubicz
Army Research Laboratory, Aberdeen Proving Ground, MD

HPC Computer Resource: SGI Origin 2000 [ARL MSRC and NRL DC], SGI PCA [ARL MSRC], SGI PCA [TARDEC DC], and Convex Exemplar [SSCSD DC]

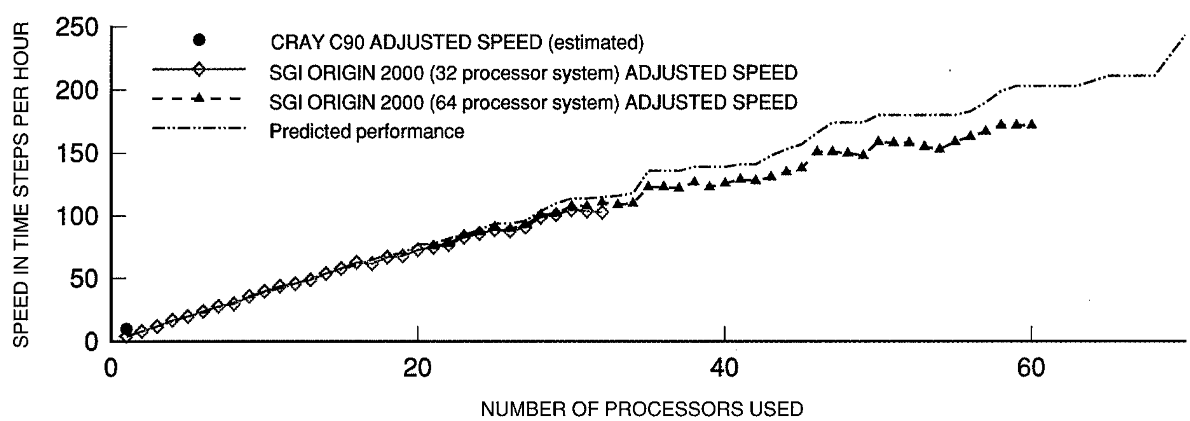
Research Objective: To reduce the cost of designing new weapon systems while improving their performance by using CFD. The long computer run-time of using CFD techniques, however, has been a major problem. As part of the CFD component of CHSSI, the well-validated code F3D was ported to a newly emerging class of parallel computers (RISC-based shared memory symmetric multiprocessors (SMPs)). This effort was aimed at simultaneously improving the performance of the code while reducing the turnaround time of the runs.

Methodology: Implicit flow solvers are an efficient method for solving CFD problems of interest to weapon systems designers. Unfortunately, there have been problems in parallelizing them. It was felt that even though SMPs have significantly fewer processors than traditional MPPs, the combination of powerful processors and aggressive efforts to tune the code would largely compensate for this limitation. Additionally, since SMPs lend themselves to the use of loop-level parallelism, it was now possible to directly parallelize vectorizable sections of code.

Results: Results on a 64-processor SGI Origin 2000 have shown speedups over one processor on a Cray C90 of up to a factor of 17 on problems ranging in size from 1 to 24 million grid points (see figure). Relative to initial efforts to run F3D on an SMP, the Origin 2000 results represent a speedup of a factor of 500 to 2,000. This confirms the importance of aggressively tuning the code. For smaller problems, the desk-side SGI Origin 200 has produced speeds comparable to that of a single processor on a C90.

Significance: The significant improvements in performance will result in a major improvement in the turnaround time for these jobs. Weapon systems designers will now be able to tackle more complicated problems than ever before, while shortening the time required to design a new system. This effort should encourage others to use these techniques in their problem domains.

JWCO: Precision Force



Performance of the two versions of the F3D code running on the platforms for which they were intended, when using a 24-million-grid-point test case

Using Electricity and Magnetism to Control Turbulence

S.H. Biringen and P.L. O'Sullivan
University of Colorado, Boulder, CO

HPC Computer Resource: Cray C90 [CEWES MSRC]

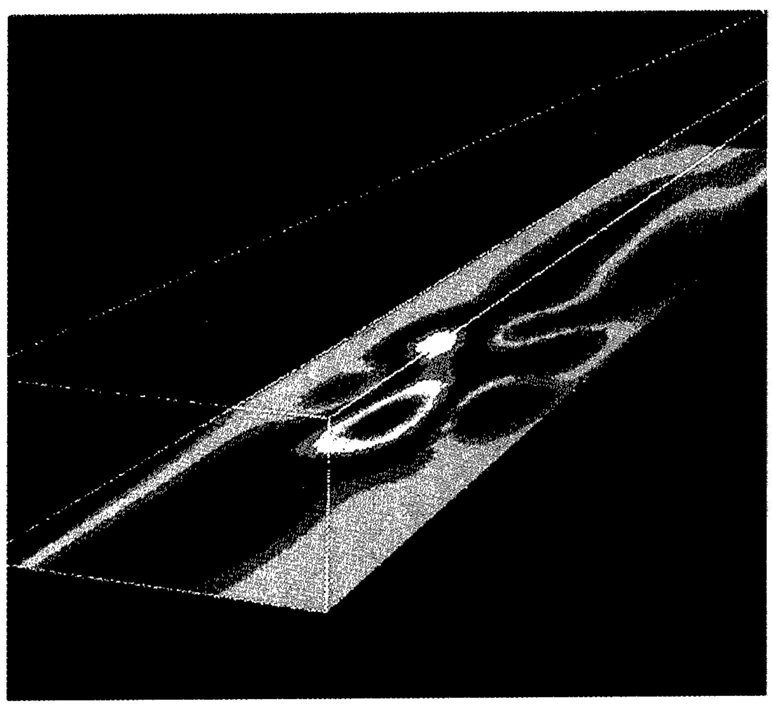
Research Objective: To investigate the possibility of using electric and magnetic fields to control turbulence and/or reduce viscous drag on sea-going vessels. Control of turbulence may lead to reduced wall pressure fluctuations and hence "quieter" operation.

Methodology: Computer simulations for a saltwater flow above a solid wall (e.g., a ship's hull in the ocean) are made by using direct numerical simulation of the governing equations. We study the flow physics of electromagnetic turbulence control (EMTC) by performing simulations in a model flow of saltwater in a rectangular channel. Computer simulations provide a complement to physical experiments in a laboratory and have the benefit of yielding detailed instantaneous flowfield information.

Results: We have simulated a novel design prototype for EMTC and found that there is scope for turbulence control. The EMTC devices are millimeter-sized electrodes and magnets embedded within the wall's surface. The force field produced by these so-called "microtiles" is sufficient to have a significant effect on the near-wall turbulent flow field, despite the very small size of the EMTC devices. Our results show that there can be localized time-average increases or decreases of 10% in the skin friction in the vicinity of a given device. The net viscous drag reduction is very small in these early simulations, but results point to the possibility of significant turbulence control with further research.

Significance: The fundamental nature of this work is valuable for obtaining concrete physical insight into the mechanisms of turbulence control. As a partner with laboratory experiments, we can provide quantitative data on the detailed interactions of the applied controlling force field and the flow turbulence. With such detail of the flow physics, we can realistically aim to provide a rational path forward in the design process (for the microtiles).

JWCO: Joint Readiness and Logistics



Time-averaged distribution of skin friction on controlled surface (red indicates an increase above the average constant skin friction in the uncontrolled case; blue indicates a local reduction)

Parallel Flow Simulations for Appended Submarines with Rotating Propulsors

R. Pankajakshan and W.R. Briley
Mississippi State University, Starkville, MS

HPC Computer Resource: IBM SP [MHPCC MSRC] and Cray T3E [NAVO MSRC]

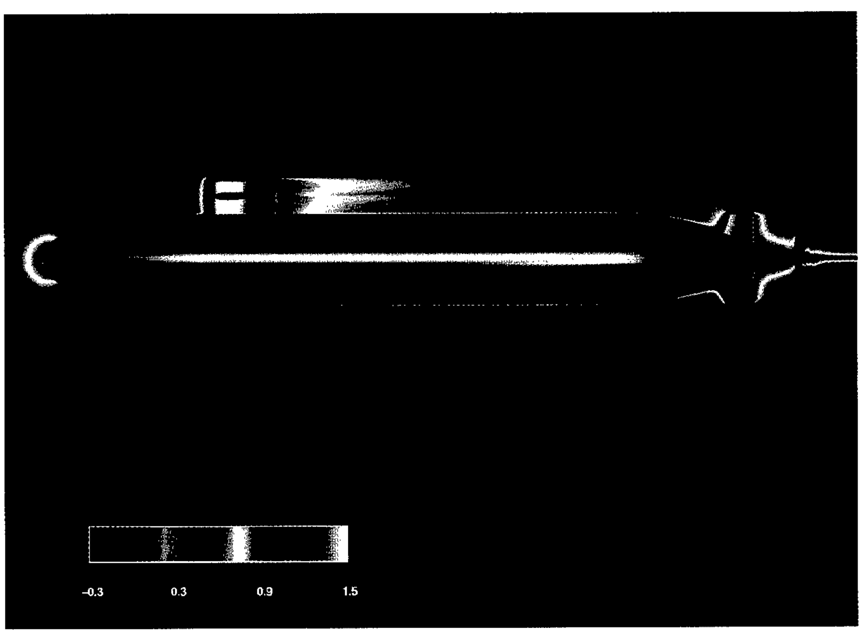
Research Objective: To use parallel computing to enable large-scale simulations for full-scale fully configured maneuvering submarines with rotating propulsors.

Methodology: Parallel supercomputing is required for large-scale computationally intensive maneuvering submarine/ propulsor simulations. A scalable parallel general multiblock incompressible viscous flow solver capable of treating complex geometries with embedded propulsors has been developed. The sequential iteration strategy for the implicit solution algorithm has been redesigned to incorporate scalable parallelism through a modified Block Jacobi Symmetric Gauss Seidel (BJ-SGS) scheme and horizontal multigrid.

Results: The parallel code has received extensive verification and validation through comparison with previous computed results and experimental comparisons from a related sequential code. A demonstration solution has been computed for a fully appended submarine configuration with rotating propulsor. This 1.6-million-point case required 57 minutes per propeller revolution (160 steps) on 51 IBM SP-2 thin nodes (1.5 GFLOPS), compared with a sequential runtime of 32 hours on an IBM-590 (43 MFLOPS). The same case required 41 minutes on a Cray T3E (2.0 GFLOPS). Scalability studies indicate that on current hardware, parallel efficiencies of 80% and more can be achieved on up to 400 processors for appropriately sized grids.

Significance: These computer simulations can result in better submarine designs as well as improved safety margins in submarines undergoing complicated maneuvers. Currently, submarine design is dependent on model-scale experiments in which some of the important flow phenomena do not scale well to full-scale conditions. These experiments can now be supplemented with physics-based computer simulations for full-scale conditions. Such computer simulations are now feasible on parallel supercomputers and can provide both quantitative analysis and improved understanding of flow phenomena affecting both design and maneuverability.

JWCO: Joint Readiness and Logistics



Axial velocity contours after 10 propulsor revolutions

Turbulent Nonlinear Free-Surface Wakes for a Combatant

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Office of Naval Research, Arlington, VA
D.G. Dommermuth
Science Applications International Corporation, San Diego, CA
E. Paterson
Iowa Institute of Hydraulic Research, Iowa City, IA
F. Stern
University of Iowa, Iowa City, IA
D.K.P. Yue
Massachusetts Institute of Technology, Cambridge, MA

HPC Computer Resource: TMC CM-5 [AHPCRC DC], Cray T90 [NAVO MSRC], and IBM SP [ASC MSRC]

Research Objective: To model and simulate details of the turbulent nonlinear free-surface hydrodynamics in the very near field of naval ships.

Methodology: This project uses leading edge computational hardware and parallel processing software to apply recently developed computational fluid dynamics algorithms and flow models with emphasis on turbulent wakes, wave breaking, and spray generation. The technical approach applies a suite of four developed computational methods to the prediction of the microscale and macroscale time-dependent hydrodynamic motions for the DDG-51 Aegis destroyer, the Navy's newest surface combatant. The four computational methods, based on unsteady Reynolds-averaged Navier-Stokes (RANS) and large eddy simulation (LES) representations of the incompressible fluid dynamic equations of motion, provide mutually collaborative and supportive techniques covering the range of scales from turbulence to ship maneuvering.

Results: Computations of the time-evolving breaking bow wave and the turbulent wake for the DDG-51 have been obtained at low resolution. New turbulence models for RANS predictions of the near-field flow based on LES computations have been produced. The turbulent far-field wake for a ship disturbance, based on a free-surface layer over an Euler bulk flow, has been computed in the time domain. Achievement of these results is the result of successful parallel computations (up to 512 nodes) and indicates the feasibility of greatly increasing the number of nodes with a corresponding reduction in computation clock time.

Significance: This research demonstrates that complex physical events on the microscale level, leading to macroscale detection, can be captured numerically with appropriate resources. This research is a composite of basic research investigations on complex hydrodynamics applied to the prediction of signature-related ship hydrodynamics.

JWCO: Precision Force, Combat Identification, Joint Readiness and Logistics

Gridless large eddy simulation computation of the turbulent bow wave on the DDG-51

Second-Order Reynolds Stress Turbulence Modeling of Three-Dimensional Oblique Supersonic Injection

Capt. C.F. Chenault, U.S. Air Force, and P.S. Beran
Air Force Institute of Technology, Wright-Patterson AFB, OH

HPC Computer Resource: Cray C90 [ASC MSRC]

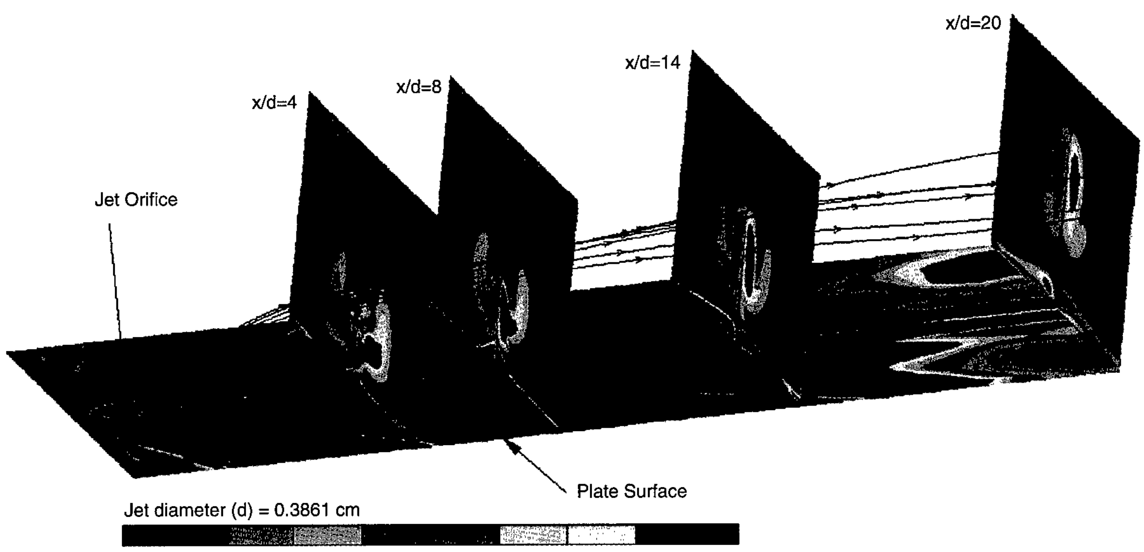
Research Objective: To validate a three-dimensional second-order Reynolds stress turbulence model (SORSTM) for the flowfield generated by supersonic injection into a supersonic wall-bounded flow at a 25-degree angle.

Methodology: The full compressible Navier-Stokes and SORSTM equations are solved with NASA Langley Research Center's FORTRAN code ISAAC. These equations are solved over a domain consisting of 3 million grid points. Numerical predictions for mean flow variables, Reynolds shear stresses, and vorticity are compared to experimental data at two downstream locations for model validation. Numerical predictions from SORSTM and an eddy viscosity model are also compared to each other to illustrate the inability of eddy viscosity models to accurately model this flowfield. Numerical predictions from SORSTM are then used to characterize a rich collection of secondary and tertiary flow structures.

Results: SORSTM predictions of mean flow and turbulent variables are in excellent agreement with experimental values. Secondary flow structures and Reynolds shear stresses are accurately captured by SORSTM, but inaccurately represented by the eddy viscosity model. As seen in the figure, SORSTM reveals a secondary flow system near the boundary layer much more complex than can be visualized experimentally. The downstream development of a primary cross-flow vortex pair is shown in the cross plane views, where the structures are observed to dominate the downstream velocity field. The protracted proximity of the primary vortex pair to the plate surface causes extensive interactions between the jet plume and the boundary layer, promoting additional turbulence and fuel/air mixing. Streamtraces of material particle paths are also shown to indicate jet penetration height.

Significance: Understanding vorticity-induced mixing of fuel and air and the thermodynamic forces acting on the solid surfaces generated by the injection process is critical to the development of SCRAMjet combustors in support of Precision Force. The present results validate a valuable tool that can provide insight to the basic vortex structures formed by supersonic injection. These results also lead to an improved understanding of experimental results and flow visualizations.

JWCO: Precision Force



Vortical structures generated by oblique supersonic injection

Shock Interaction with a Turbulent Premixed Flame During a Deflagration-to-Detonation Transition

A.M. Khokhlov, E.S. Oran, and E.I. Stefani
Naval Research Laboratory, Washington, DC

HPC Computer Resource: Cray C90 [ASC MSRC]

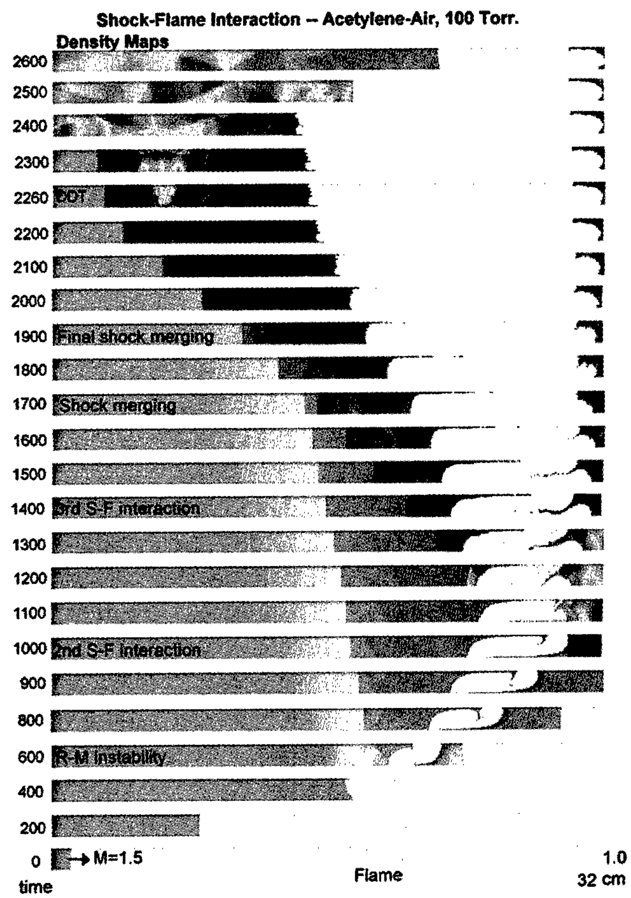
Research Objective: To study the amplification of turbulent burning by shock-turbulent flame interactions during the process of deflagration-to-detonation transition (DDT). Understanding and controlling DDT can prevent and mitigate the effects of hazardous accidents in civilian and military systems (such as aircraft carriers and mines).

Methodology: The numerical model solves multidimensional time-dependent Navier-Stokes equations plus equations describing chemical heat release and volume heat losses. The fluid part of the equations is solved by using a high-resolution Godunov-type numerical scheme that incorporates a Riemann solver. Fluxes due to thermal conduction, diffusion, and viscosity effects are evaluated using central differencing and are added to the numerical fluxes. Chemical reaction and heat losses are added to the model using time-step splitting. A fully threaded tree (FTT) adaptive mesh refinement algorithm is incorporated to increase both spatial and temporal resolution of the model at shocks, flame fronts, and other regions of high spatial gradients.

Results: Numerical simulations for an acetylene-air mixture at 100 torr demonstrated that the coupling takes place via a high-amplitude acoustic field that is generated during multiple interactions of a flame with reflected shocks. Both experiments and analyses indicate that this coupling strongly depends on the system's reactivity.

Significance: Deflagration-to-detonation transition is the unsteady process by which a high-speed turbulent flame, or deflagration, becomes a powerful supersonic reaction wave, or detonation. Unwanted DDT in military systems, such as aircraft carriers, and in civilian aircraft causes human and equipment losses. Equipment losses alone, such as occurred on the USS *Iowa*, run into billions of dollars. An understanding of the basic, controlling parameters for DDT is crucial for the design of engines for high-speed flight, conventional explosives, and maintaining safe operating conditions in regions near explosives and energetic gases. Because of the unsteady nature of DDT, accurate experimental results are extremely difficult to obtain. These HPC simulation results describe shock-amplified turbulent burning, and relate the conditions required for DDT to the geometry of the confinement, strength of the incident shock, and the properties of the flammable mixtures.

JWCO: Joint Theater Missile Defense, Military Operations in Urban Terrain, Joint Readiness and Logistics



Time history of shock-flame interaction showing DDT in acetylene-air system at 200 torr pressure

Dynamics of Supersonic Inlets: Shock/Turbulent Boundary Layer Interactions

D.V. Gaitonde and J.S. Shang
Air Force Research Laboratory, Wright-Patterson AFB, OH

HPC Computer Resource: Cray C90 [CEWES and NAVO MSRCs]

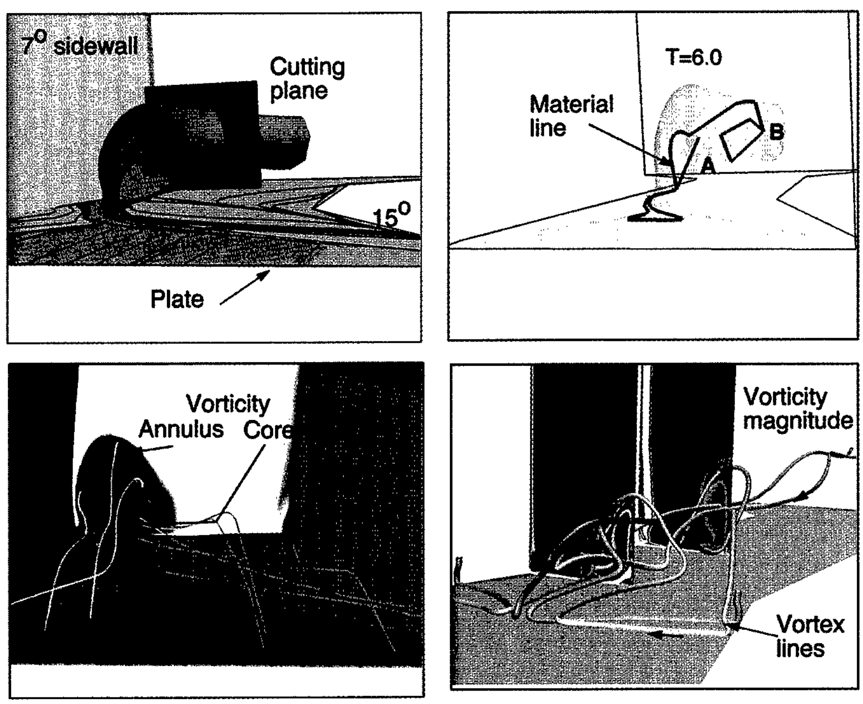
Research Objective: To elucidate the behavior of the mean flow in a simulated inlet. Flow compression and deceleration are an essential precursor to combustion in inlet systems. In supersonic flight, the consequent interaction between the shock wave and the boundary layer degrades propulsion system performance by causing three-dimensional (3-D) separation. The structure of highly asymmetric interactions is investigated and the computations are used to characterize the effect of increased compression on inlet distortion.

Methodology: The numerical model consists of the full 3-D mean compressible Navier-Stokes equations in strong conservation form and mass-averaged variables. The FDL3DI code is used in which inviscid fluxes are evaluated to nominal third-order accuracy with Roe's flux-difference split scheme, with a limiter for monotonicity. Viscous terms are differenced to second-order accuracy in a centered manner. The effects of turbulence are incorporated through the eddy viscosity assumption coupled with a two-equation model with low-Reynolds-number terms and a compressibility correction.

Results: The graphic summarizes various aspects of the findings. The vortical structure in asymmetric interactions impinges on and subsequently aligns parallel to the side wall. This dominant feature essentially reorganizes the incoming boundary layer into an internal core and an outer annulus region. Increasing compression strength causes a significant enhancement of longitudinal vorticity and is accompanied by a complex sequence of bifurcations leading to full 3-D separation.

Significance: The work provides a new unified description of shock, streamline, and vorticity fields that significantly increases basic understanding of high-speed inlet design and performance. At conditions of asymmetry, the sidewall-vortex interaction causes much higher loading on the surfaces. The improved understanding of the rotational dynamics reveals a rich structure not previously recognized.

JWCO: Precision Force, Joint Theater Missile Defense



Top left: Separated boundary layer surface causes wall-vortex interaction.
Top right: Motion of material line in mean flowfield indicates origin of fluid-forming core.
Bottom left: Computations provide unified understanding of streamline and vorticity fields.
Bottom right: Increasing compression results in more longitudinal vorticity.

Analysis of Advanced Fighter Auxiliary Power Unit Exhaust Impingement

Capt. P.M. Cali, U.S. Air Force
Air Force Research Laboratory, Wright-Patterson AFB, OH

HPC Computer Resource: Cray C90 [CEWES and NAVO MSRCs]

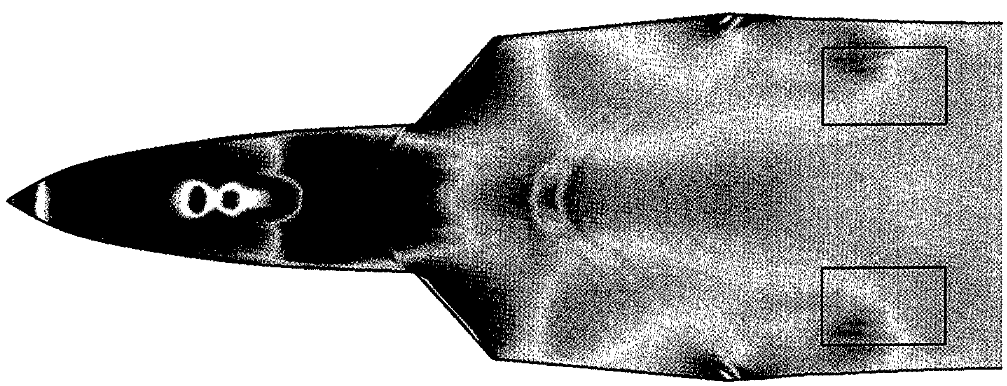
Research Objective: To analyze the exhaust flow associated with the auxiliary power unit (APU) of an advanced fighter aircraft to assess the level of surface heating on the fuselage adjacent to the exhaust port.

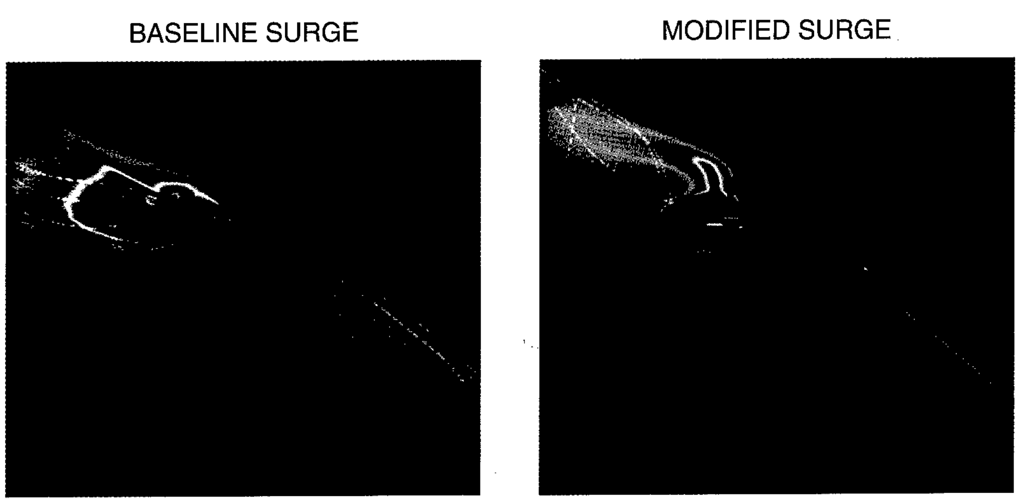
Methodology: Three-dimensional, compressible Navier-Stokes equations were solved on a Chimera grid domain. The flow solver FDL3DI is an implicit, approximately factored, finite-difference algorithm of Beam and Warming. The grid was created with GRIDGEN, and PEGSUS was used to calculate intergrid communications.

Results: Calculations were made with the surge (high pressure air vent) line in both its original location and a modified location. Temperature distribution and characteristic streamlines in the region of the APU are shown for each case. In the baseline case, the interaction between the external flow and the APU exhaust creates a large inward component of the flow. This inward flow sweeps the hot exhaust gases inboard and results in a high-temperature region adjacent to the APU exhaust port. Relocating the surge line to an inboard position diverts the flow downstream away from the vulnerable area.

Significance: The extent of the temperature footprint inboard of the exhaust port in the modified case is vastly reduced. At approximately two diameters downstream of the exhaust port's leading edge, there is a 40% reduction in the temperature on the aircraft skin.

JWCO: Precision Force





Deployed APU showing streamlines and temperature contours with baseline surge line location and modified surge line location

Dynamic Stability of Vehicles Carrying Bulk Liquid

S.K. Aliabadi and T.E. Tezduyar
Army High Performance Computing Research Center Minneapolis, MN

HPC Computer Resource: Cray T3D [AHPCRC DC]

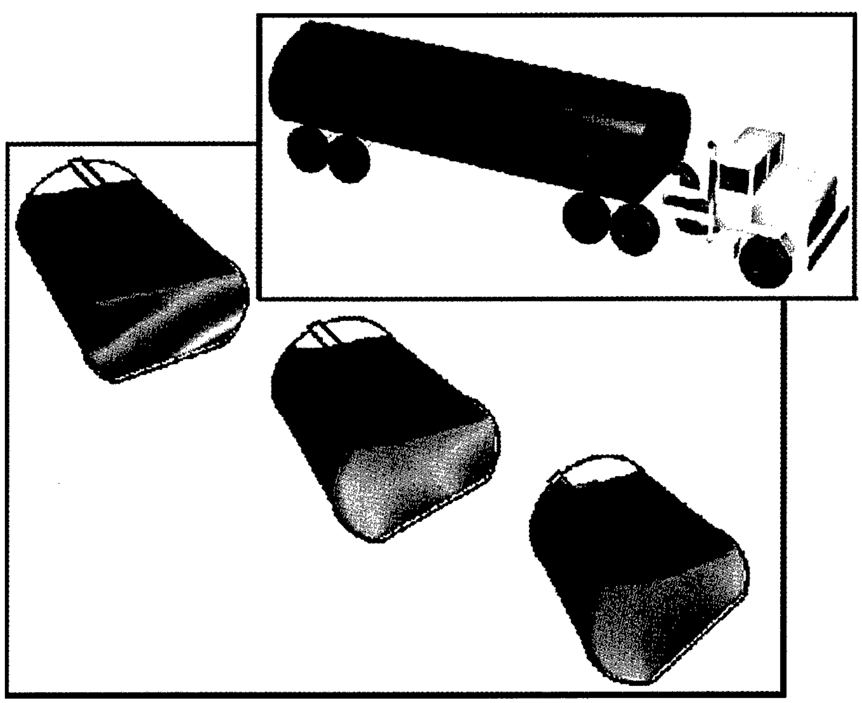
Research Objective: To develop computational tools and numerical methods to accurately simulate incompressible two-phase flow problems. One of the applications of two-phase flow is the instabilities caused by sloshing in a bulk liquid transport vehicle.

Methodology: A stabilized finite-element formulation with a fixed mesh is developed to simulate two-phase flow problems. This formulation is implemented on the Cray T3D and Cray T3E parallel computers. The mathematical model is based on the Navier-Stokes equations coupled to an advection equation governing the interface function. The interface function with two distinct values representing two fluids is advected throughout the computational domain with fluid velocity. Three-dimensional rigid-body dynamic equations are also coupled to the finite-element formulations and solved simultaneously for the motion of the tanker truck as function of time. The fluid dynamics equations are written in a non-inertial frame to account for this motion. The finite-element mesh used consists of 343,560 hexahedral elements and 357,911 nodes. At each time-step, a coupled system of nonlinear equations with 1,704,661 unknowns is solved.

Results: The method has been applied to simulate liquid sloshing in a partially filled tanker truck driving over a bump. The suspension system of the truck absorbs the initial displacement due to the bump and transfers the generated forces to the structure of the truck.

Significance: It is only because of the efficient parallel implementation and the computational capability offered by the new generation of parallel computers that large-scale unsteady three-dimensional simulations are feasible. The parallel computations allow problems with large numbers of degrees of freedom to be solved with greater accuracy than was previously possible. Results of these simulations help design new, safer tanker trucks.

JWCO: Military Operations in Urban Terrain, Joint Readiness and Logistics



Motion of the truck, sloshing, and fluid pressure at different instants

Free-Surface Flow Past a Cylinder

I. Guler, M. Behr, and T.E. Tezduyar
Army High Performance Computing Research Center, Minneapolis, MN

HPC Computer Resource: TMC CM-5 [AHPCRC DC]

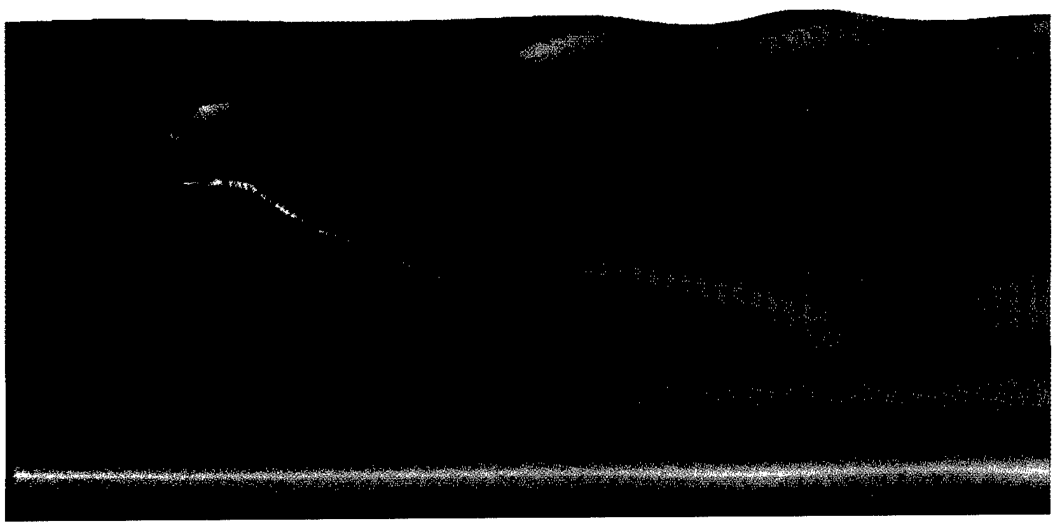
Research Objective: To develop computational techniques for simulating the free-surface flows around surface-piercing bodies. In these problems, the location of the free-surface is not known a priori and needs to be determined as part of the overall solution.

Methodology: Three-dimensional Navier-Stokes equations for incompressible flow are discretized by using a stabilized space-time finite-element formulation for deforming spatial domains that automatically takes into account the motion of the free surface. The free-surface height governed by kinematic free-surface condition is also solved with a stabilized formulation. Mesh update is achieved with a special-purpose mesh moving scheme.

Results: Free-surface flow past a cylindrical support is simulated at a Reynolds number 10 million based on the cylinder diameter and an upstream Froude number 0.564. The finite-element mesh used in this computation consists of 230,480 triangular-based prism elements and 258,764 space-time nodes. The bow wave in front of the cylinder, the hydraulic jump behind, and the V-shaped waves in the wake are characteristics of this flow problem.

Significance: The capability of numerically simulating free-surface problems involving surface-piercing bodies provides a new tool to study the flow structure and wave pattern around bridge piers, offshore platform legs, and submarine periscopes.

JWCO: Joint Readiness and Logistics, Precision Force



Computed wave pattern at an instant. Free surface is color-coded with the velocity magnitude; side boundary surface is color-coded with the fluid pressure.

Nonlinear Dynamic Fluid-Structure Interaction

Maj. S.A. Morton, U.S. Air Force, and R.B. Melville
Air Force Research Laboratory, Wright-Patterson AFB, OH

HPC Computer Resource: Cray C90 [ASC MSRC] and Cray T916 [ARL MSRC]

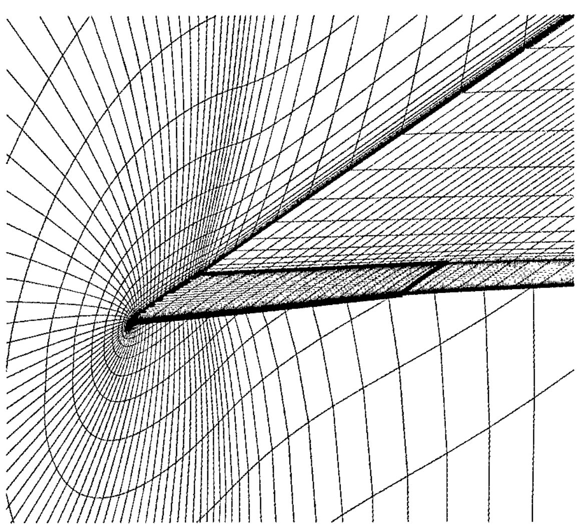
Research Objective: To develop a highly accurate and cost-effective dynamic aeroelasticity simulation capability for fluid structure interaction on complex configurations.

Methodology: A high-fidelity, implicit fluid dynamics solver is coupled with a structural solver and a general grid deformation solver and a general grid deformation capability to allow simulation of flow over flexible geometries in a complex, overset grid system. The solvers are applied iteratively so that the fluid and structure states are synchronized in time without lag, allowing higher order temporal accuracy to be achieved. The method is well-suited to nonlinear regimes including high angle-of-attack separated flows and transonic shock-boundary layer interactions that cannot be simulated accurately with traditional linear aeroelasticity methods.

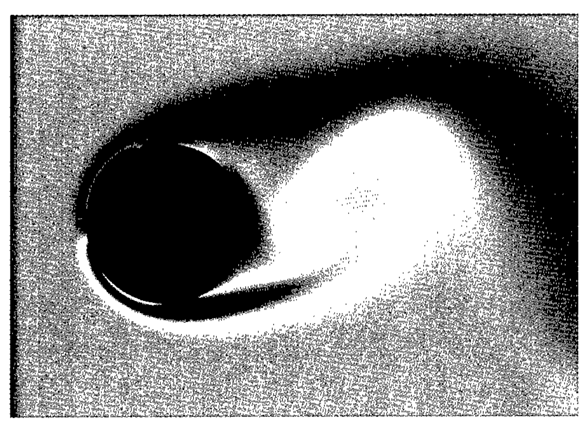
Results: The aeroelastic simulation capability has been validated on two benchmark applications. The motion of an elastically mounted cylinder, with its highly nonlinear, separated flow, was resolved to second-order accuracy; it compared well with experiments and other simulations. Additionally, both static deflections and unsteady, transonic wing flutter were captured for the AGARD 445.6 wing. Increases in temporal accuracy yielded an order-of-magnitude improvement in simulation efficiency for highly nonlinear flows.

Significance: The development of a robust and reliable aeroelastic simulation capability will allow reduced dependence on costly wind-tunnel and flight testing for new and modified aging aircraft, as well as existing aircraft with new store configurations. This tool is vital to understanding the fundamental interactions between nonlinear flow and air vehicle structures in the flight envelopes in which Air Force fighters, bombers, and transports routinely fly. Flexible weapon systems will be affected by improved performance and less susceptibility to flutter and buffet.

JWCO: Precision Force



Grid topology of the AGARD 445.6 wing



Vorticity contours of an elastically mounted cylinder in motion

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Computational Chemistry and Materials Science

Computational Chemistry and Material Science (CCM) is the most fundamental area within the High Performance Computing Modernization Program. The chemical and material properties derived through CCM are often cornerstones upon which research and development in other computational technology areas are built.

The 15 CCM success stories that follow illustrate the broad range of DoD warfighting problems that are being addressed with CCM methods. The first three stories summarize CCM efforts in the Army to better understand the chemical and dynamic processes in high-energy explosives. These computations provide heretofore-unavailable insights into how explosives work and guide the design of safer, higher power, insensitive munitions. The next three stories also deal with the computational design of new high-energy materials, highlighting Air Force programs to develop high-energy rocket propellants for the Integrated High-Payoff Rocket Propulsion Technology initiative, a joint DoD/NASA/industry program to double the nation's rocket propulsion capabilities by the year 2010. Stories 7 through 11 show the great breadth of CCM projects in DoD that are focused on developing new electromagnetic materials for warfighting applications. Stories 7 and 8 use CHSSI software to understand mechanisms of laser resistance in organic materials to design laser-hardened aircraft canopies and other pilot-protection measures. The next three stories describe CCM modeling aimed at designing new semiconductors, superconductors, and conducting polymers for the advanced high-performance electronics that will be necessary for 21st century aircraft, satellite, and sensor technology. Stories 12 and 13 exemplify Navy and Air Force efforts to develop new structural materials, both metal alloys and advanced polymers. These projects are typical of efforts to develop new materials that will withstand the extremely oxidizing/high-temperature environments of future jet aircraft and rocket engines. The final two success stories show how CCM is used to understand the chemistry of hazardous materials in the environment, both for developing remediation strategies for base clean up and devising methods to efficiently dispose of our chemical weapons stockpiles. The data acquired from these projects will feed into environmental quality models to improve DoD's ability to predict the long-term effects of hazardous wastes on communities near DoD installations.

Major Scott G. Wierschke, USAF
Air Force Research Laboratory
Edwards Air Force Base, CA
CTA Leader for CCM

Desensitization of Detonable Material

B.M. Rice, W. Mattson, and S.F. Trevino
Army Research Laboratory, Aberdeen Proving Ground, MD

HPC Computer Resource: SGI PCA [ARL MSRC]

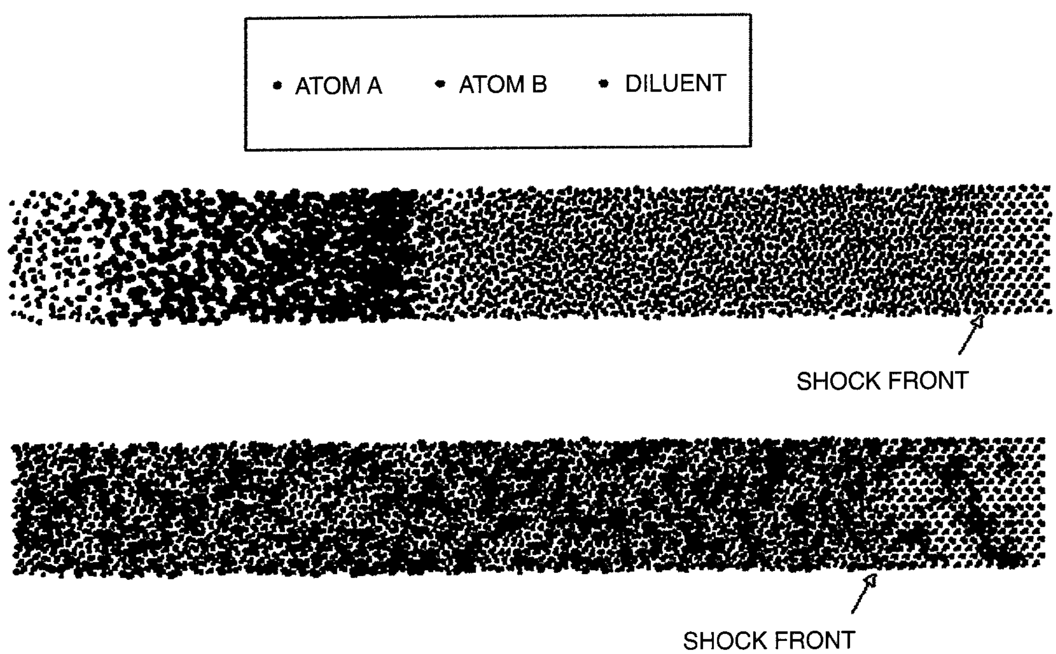
Research Objective: To exploit information obtained from earlier molecular dynamics simulations of detonation to tailor explosives with desired detonation characteristics. In this application, we investigate two tailored explosives—one that will not initiate and the other that will quench a detonation once the reaction wave is initiated.

Methodology: Molecular dynamics simulations, based on classical mechanical equations of motion, are used to simulate the behavior of tailored explosives subjected to shock initiation by flyer plate impact. Molecular species behind the shock wave are monitored to determine the degree of reaction and whether detonation is sustained. Results are interpreted in terms of the tailoring guidelines that were extracted from the previous molecular dynamics studies of pure explosive. The magnitude of the systems undergoing simulation and the corresponding CPU requirements use many-body molecular dynamics algorithms developed for multiprocessing on the ARL MSRC SGI Power Challenge Array. The algorithms developed for these simulations are being generalized and incorporated into the classical molecular dynamics package in the CCM CHSSI program.

Results: Detonation was quenched in a pure explosive after the energy of a shock wave was attenuated from traversing a 100-Å-wide slab of inert, heavy diluent (upper frame of figure). Detonation was reestablished for shock waves crossing diluent slabs with smaller widths. Detonation was found to occur for solid solutions of explosive with concentrations of inert diluent of 34.4% or less; detonation could not be initiated for higher concentrations of diluent (lower frame of figure).

Significance: This study has shown that results obtained from molecular simulation can be used in the design of materials with specific performance objectives—in this case, desensitization of detonable material. The previously reported molecular dynamics simulations of detonation of the pure explosive established the reaction mechanisms of the explosive, and the study reported here explored manipulations of the materials to affect those reaction mechanisms. The study has clearly shown that microscale information can be used successfully to design explosives with desired detonation characteristics.

JWCO: Precision Force



Upper frame: Tailored explosive in which detonation wave is quenched upon traversing a layer of inert diluent. Species to the left of diluent slab are detonation products, and species to the right of diluent slab are unreacted explosive. Lower frame: Tailored explosive consisting of solid solution of explosive and inert diluent. This solution does not sustain a detonation. Although crystal lattice is disrupted by shock wave, no products are formed.

Quantum Mechanical Investigations of Solid Explosive Under High Pressure

B.M. Rice and G. Krasko
Army Research Laboratory, Aberdeen Proving Ground, MD

HPC Computer Resource: SGI PCA [ARL MSRC]

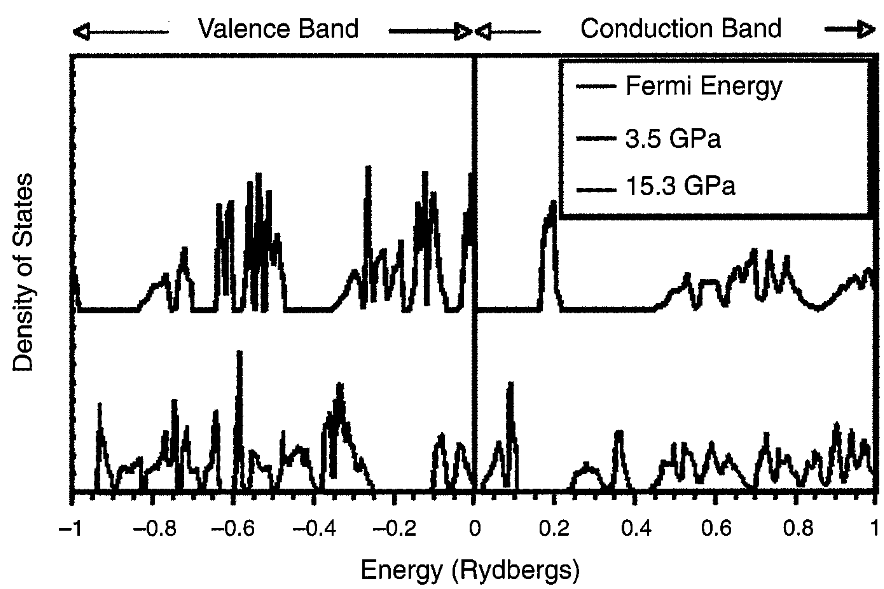
Research Objective: To investigate the effect of pressure on the electronic structure of an explosive. The results will address the recently proposed theory that the initiation of detonation is due to pressure-induced metallization/atomization of the explosive rather than more traditional views (thermal activation or mechanical fracture).

Methodology: First principles calculations, including pseudopotential and linear muffin-tin-orbital (LMTO) methodologies are used to predict transitions from the ambient phase of a prototypical energetic molecular crystal for a variety of high hydrostatic pressures.

Results: Quantum mechanical calculations of crystalline nitromethane arranged in geometries consistent with measured structures up to15 GPa have clearly shown the closure of the insulator band gap of electronic states (see figure). The closure indicates that bonding electrons within this explosive have delocalized (metallization), and reactive fragments of the previously intact molecule have formed. In a pressure wave of an explosive, these nascent fragments are free to react with accompanying energy release to drive a detonation.

Significance: This work indicates that models used in earlier molecular simulations of detonation are reasonable and that metallization cannot be eliminated from consideration as the key mechanism for initiation to detonation. In view of these results, it is imperative that the phenomenon of detonation be re-examined according to this new mechanism.

JWCO: Precision Force



Band structure of the explosive nitromethane at 3.5 GPa (upper curve) and 15 GPa (lower curve). The Fermi energy is the point that separates the valence band from the conduction band. The insulator gap is the distance between the highest-energy valence band and the lowest-energy conduction band.

Characterizing the Dark Zone of Nitramine-based Gun Propellants Through Quantum Mechanics

S.W. Bunte, B.M. Rice, and C.F. Chabalowski
Army Research Laboratory, Aberdeen Proving Ground, MD

HPC Computer Resource: SGI PCA [ARL MSRC]

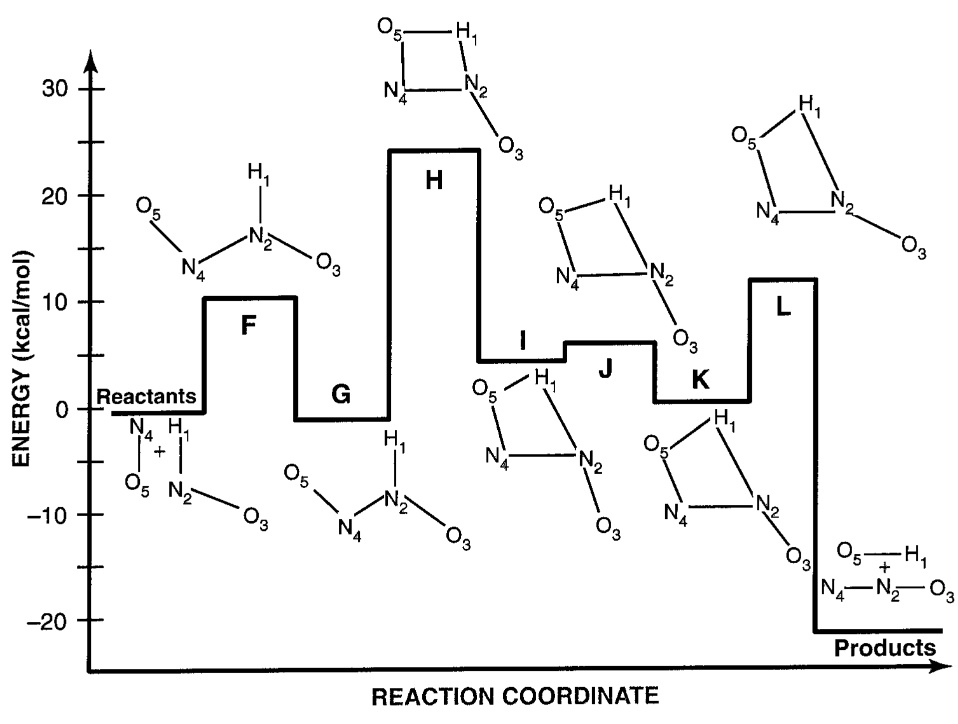
Research Objective: To characterize the potential energy surface of reactions deemed to be important in the chemistry of nitramine-based gun propellants.

Methodology: Quantum mechanical calculations at the quadratic interaction including single and double substitution (QCISD) level were used to locate and characterize critical points for two reaction paths on the HNO + NO → N_2O + OH potential energy surface. These high-level calculations were required after determining that similar calculations using a lower (and commonly used) level of quantum mechanical theory predicted significantly different results.

Results: Two completed reaction pathways for the HNO + NO → N_2O + OH reaction have been determined and confirmed by geometry optimizations and vibrational frequency analyses, followed by intrinsic reaction coordinate calculations. Path 1 includes three activation barriers—the largest of which is approximately 50 kcal/mol. The magnitude of this barrier precludes this path as a contributor to thermal reaction under combustion conditions. The height of the largest energy barrier on Path 2 is 24 kcal/mol, which is in quantitative agreement with the activation energy predicted through analyses of experimental data.

Significance: A distinctive feature observed during the combustion of nitramine containing solid gun propellants is the two-stage nature of the flame. At pressures around 2 MPa, there is a nonluminous region in the flame, commonly referred to as the dark zone. The dark zone is known to contain NO and NO-containing intermediates that react slowly. Detailed kinetic modeling, coupled with sensitivity analyses of possible reactions, indicate that the HNO + NO reaction is the most sensitive in controlling the ignition chemistry of nitramine propellants. It is the rate-controlling step in the thermal reduction of NO by H_2 at temperatures greater than 1000 K and is also known to initiate the formation of N_2 and H_2O. Quantitative determination of the kinetic parameters for this reaction is crucial in establishing the database needed to model the combustion of nitramine-based gun propellants.

JWCO: Precision Force



Zero-point corrected relative energies (kcal/mol) of critical points on the low energy pathway for the reaction HNO + NO → N_2O + OH

Calculation of the Heats of Formation of Prospective Rocket Fuels

J.D. Mills and J.A. Boatz
Air Force Research Laboratory, Edwards AFB, CA

HPC Computer Resource: IBM SP [MHPCC DC and ASC MSRC]

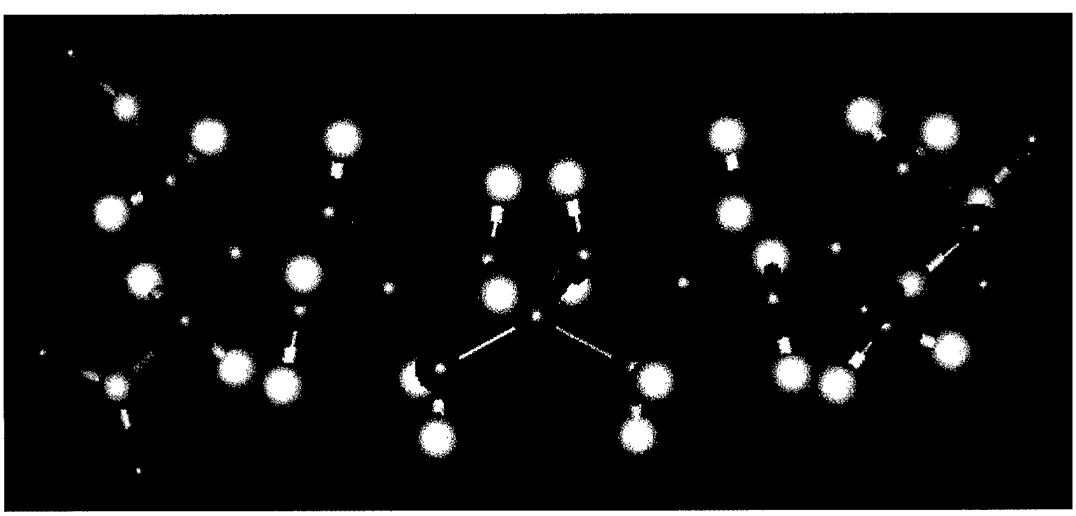
Research Objective: To accurately predict the heats of formation on the energy content of proposed propellants. Since synthesis of even small quantities of novel chemical compounds can be extremely resource intensive, it is desirable to narrow the search for new energetic fuels and fuel additives to only those candidates that show particular promise. Calculational methods must not only be affordable and timely but of sufficient accuracy to ensure the reliability of performance predictions based on their results.

Methodology: The GAMESS computer program was used to perform a series of calculations based on semi-empirical considerations as well as quantum chemical first principles. On the parallel IBM SP machines at the Maui High Performance Computing Center and the Air Force Aeronautical Systems Center, quick turnaround and high throughput were enabled by the efficient scalability implemented in the code. Heats of formation were derived both from the energies of the target molecules alone, as well as by making use of what are termed isodesmic or bond-preserving reactions. Therefore, the modest errors implicit in the calculation are expected to cancel in the subtraction of reactant and product energies.

Results: The gas-phase heats of formation of eight unusual strained and substituted organic molecules ranging in size from C_6H_8 to $C_{17}H_{24}N_4O_8$ were determined using a number of methods. It was found that a relatively high level of theory applied to appropriate isodesmic reactions is necessary to surpass the accuracy of wholly empirical prescriptions that are based on the approximate transferability of chemical-functional-group energetics between different molecules and that involve almost no computation.

Significance: These calculations provided critical parameters necessary to evaluate a specific set of proposed rocket fuels and also help to justify a means of efficiently screening prospective molecules in the future. Theoretical investigations of this sort, in conjunction with experimental research, are part of the effort to reduce the time and expense required to develop and deploy new propellants capable of higher performance and increased payload. The investigations, therefore, have a role in the improvement of space-based intelligence gathering necessary for information superiority, prompt and efficient logistical deployment and remote force projection, and other commercial and military space-launch needs.

JWCO: Information Superiority; Joint Readiness and Logistics



The HF(6-31G(d)) optimized geometry of $C_{17}H_{24}N_4O_8$ (black: carbon; yellow: hydrogen; blue: nitrogen; red: oxygen)

Design of New, High-Energy Species

M.S. Gordon
Iowa State University, Ames, IA

HPC Computer Resource: IBM SP [MHPCC DC]

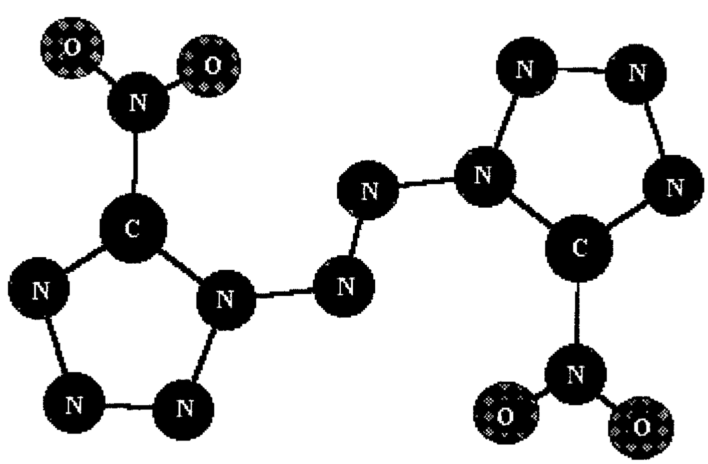
Research Objective: To develop new fuels with much higher specific impulse than the standard LOX/LH2. The goal is to put together an array of powerful tools in theoretical chemistry to design new, high-energy species and to provide potential synthetic routes to obtain these species.

Methodology: A combination of the highly accurate G-2 model with homodesmic reactions is being used to determine the heats of formation for potential high-energy species. These computed heats of formation are then used to predict the specific impulse for each species. The quantum chemistry codes GAMESS and ACESII have been used to perform the calculations. The parallel features of GAMESS have been essential for the success of this project.

Results: The molecular geometry of the polynuclear, high nitrogen-content (10 nitrogens in a row!) species shown below has been determined using second-order perturbation theory. The subsequent computation of the vibrational frequencies provides the information necessary to calculate the heat of formation of this compound, using the methods outlined above. The resulting heat of formation is 457 kcal/mol. This leads to a specific impulse of 329 s, considerably better than that for hydrazine (240 s) and also better than the combination LOX/RP1 (300 s). Therefore, this species is a very promising, high-energy density matter candidate.

Significance: High-energy species with specific impulses exceeding those of currently used propellants offer substantial savings in launch costs. Since rocket propellants typically account for approximately 80% of the total mass of a rocket, any increase in propellant efficiency can result in larger payloads and other cost savings. Furthermore, high-energy molecules with a high nitrogen content such as the one shown below are more environmentally benign than, for example, ammonium perchlorate (AP)-based solid propellants currently in use today.

JWCO: Joint Readiness and Logistics, Joint Theater Missile Defense



SCF/6-31G(d) optimized geometry

Simulating High-Energy Density Rocket Fuels

M. Pavese, S. Jang, S. Jang, and G.A. Voth
University of Utah, Salt Lake City, UT

HPC Computer Resource: IBM SP [MHPCC DC and ASC MSRC]

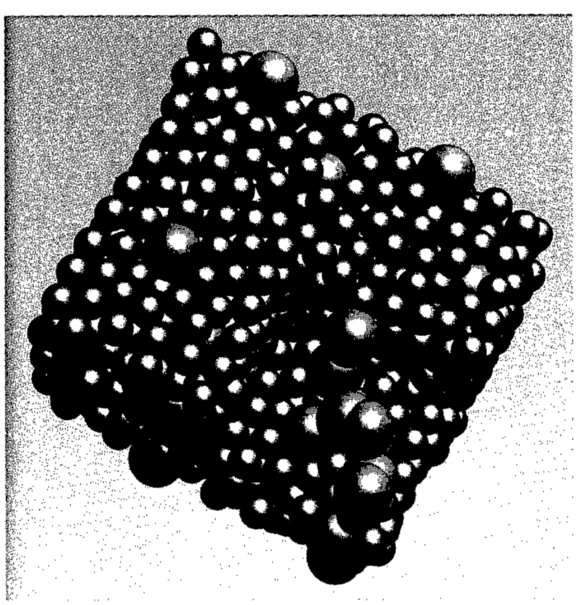
Research Objective: To understand the dynamical processes occurring in low-temperature solid hydrogen, especially containing lithium impurities. Solid hydrogen is commonly used as rocket fuel. Doping the solid hydrogen with atomic impurities promises to improve its performance. However, there is a large thermodynamic driving force for their recombination. A detailed picture of this process and how it might be prevented is required before this fuel can be developed.

Methodology: We have used simulation techniques that incorporate quantum effects in many-body systems to allow us to obtain reliable results. The centroid molecular dynamics (CMD) method has been developed to calculate the approximate time evolution of many-body quantum mechanical systems such as those encountered in the present simulations. This method has natural features that lend it to parallel computation, and we have exploited those features to develop a highly parallel algorithm for doing finite temperature quantum dynamics. Each one of a primary set of processors has a subgroup of processors working under it. In this scheme, communication overhead is kept very low, resulting in almost 90% efficiency on 64 nodes of the IBM SP.

Results: We first calculated the bulk phonon spectrum of solid para-hydrogen at 4 K to see if we could correctly describe the lattice vibrations. The results are in good agreement with experiment, predicting peaks in the spectrum in the range of 60-80 cm^{-1}. In classical simulations, peaks appear in the spectrum out to 150 cm^{-1}, a region where no phonons have been found experimentally. Next, we determined the free energy barrier to recombination of two lithium impurities (which is close to 80 times the thermal energy at 4 K). More recently, we have investigated the limit on the possible maximum doping concentration of lithium atoms before recombination becomes immediate. Initial results indicate that this occurs above 3 mol percent doping. It proceeds by a mechanism of initial creation of lithium dimers, which releases heat as well as creating free volume for the hydrogen to reorganize. Recombination of the rest of the lithium atoms follows soon after this step.

Significance: This research is important for the eventual enhancement of space lift capacity of the Air Force, thus positively impacting warfighting capabilities while reducing costs. The impact on promoting basic research is also positive since this simulation methodology is highly nonstandard.

JWCO: Joint Theater Missile Defense



Simulation of solid para-hydrogen (small purple spheres) doped with atomic lithium impurities (larger orange spheres) at 4 K. The doping level is 3.3 mol percent. In the lower right, a section of the hydrogen has been cut away so that the progress of the lithium recombination can be seen more clearly.

DoD Challenge Application: Materials for Laser Hardening

Z. Wang, P.N. Day, and R. Pachter
Air Force Research Laboratory, Wright-Patterson AFB, OH

HPC Computer Resource: IBM SP [ASC MSRC]

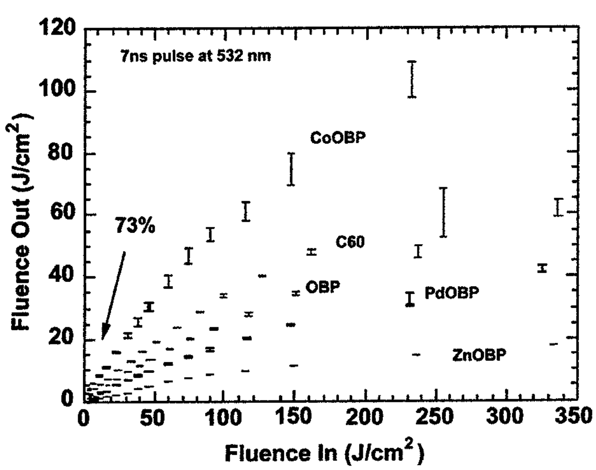
Research Objective: To explore and design novel materials with controlled properties for laser-hardening applications by applying newly developed methods, algorithms, and scalable advanced software. In particular, we study materials with fast nonlinear optical (NLO) response over broad spectral bandwidths such as reverse saturable absorbers, as well as polymer-dispersed liquid crystals and advanced absorbing dyes, which are critical for laser eye and sensor protection.

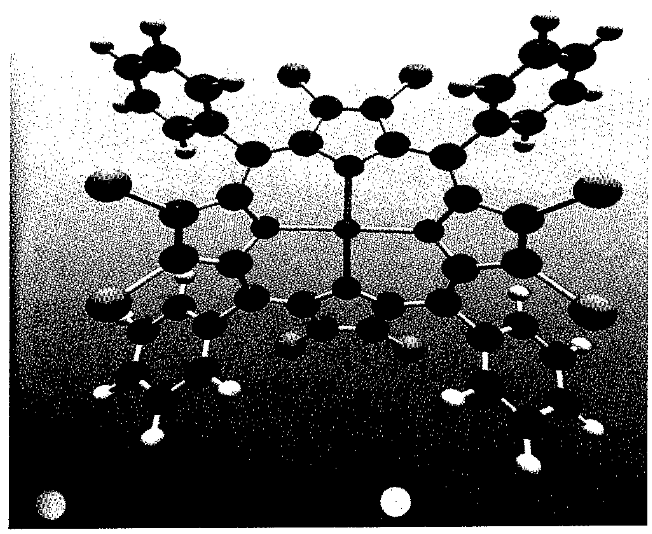
Methodology: First-principle calculations are carried out using a suite of scalable quantum chemistry codes (GAMESS) and atomistic simulations with the fast molecular dynamics (FMD) code, including a three-dimensional fast multipole method to address long-range electrostatic interactions. GAMESS and FMD are CCM CHSSI projects.

Results: The behavior of complex organometallic materials was modeled using a combination of electronic structure and solvation effective fragment potential method calculations. Porphyrin derivatives were studied to assess their optical-limiting potential, such as Zn tetraphenyl-octobromyl-porphyrin. A study of porphyrins with meso-acetylene substituents has been carried out. The calculated electronic structures clearly show that the acetylene group contributes to the π-electron conjugation along the porphyrin ring consistent with experimental results. The results for phthalocyanines indicate that the H_2 and Cu phthalocyanines are planar, while the Pb and Sn phthalocyanines are nonplanar, and the effects of puckering on the absorption spectra were evaluated. Good agreement with the experimental spectra was observed. These fundamental advances provide the basic understanding and means for effective and efficient design of laser-hardened materials and guide exploratory and advanced development programs.

Significance: The molecular design of novel materials, enabled by reliable properties predictions using extensive HPC, is crucial for DoD laser-hardening applications that address critical warfighting needs. Moreover, these applications, combined with the innovative use of HPC through our CHSSI efforts for the ab initio GAMESS and molecular dynamics FMD codes, show potential for significant progress in materials design to affect the scientific community as a whole.

JWCO: Electronic Combat





Experimental optical-limiting comparison; zinc tetraphenyl-octobromyl-porphyrin (ZnOBP).

Modeling of Materials in Solution

P.N. Day and R. Pachter
Air Force Research Laboratory, Wright-Patterson AFB, OH
J.H. Jensen and M.S. Gordon
Iowa State University, Ames, IA

HPC Computer Resource: IBM SP [ASC MSRC]

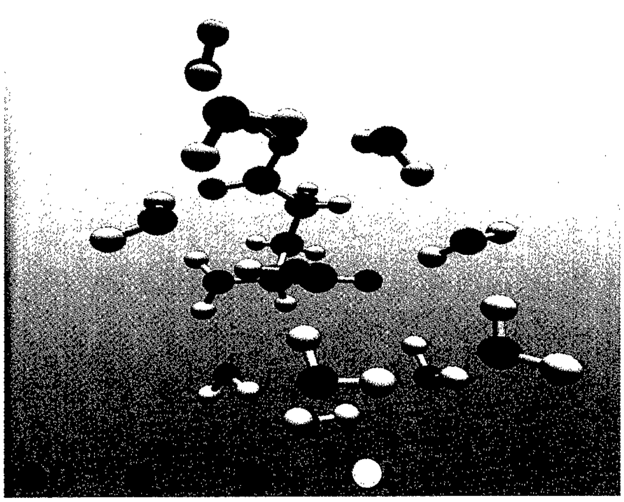
Research Objective: To further develop the effective fragment potential (EFP) methodology and scalable computer software to enable a reliable prediction of the behavior of a complex material in solution.

Methodology: A broad class of materials that are being considered for laser-hardening applications exists in solution or gel form. The inclusion of solvent effect interactions is therefore essential. Ab initio calculations were carried out using parallel GAMESS, where the EFP routines are incorporated. The EFP technique enables the inclusion of discrete solvent molecules in an ab initio method without the computational expense of a full ab initio super-molecule calculation. Modeling of various solvents was recently included with the development of transferable exchange repulsion potentials. This effort is part of a CHSSI project.

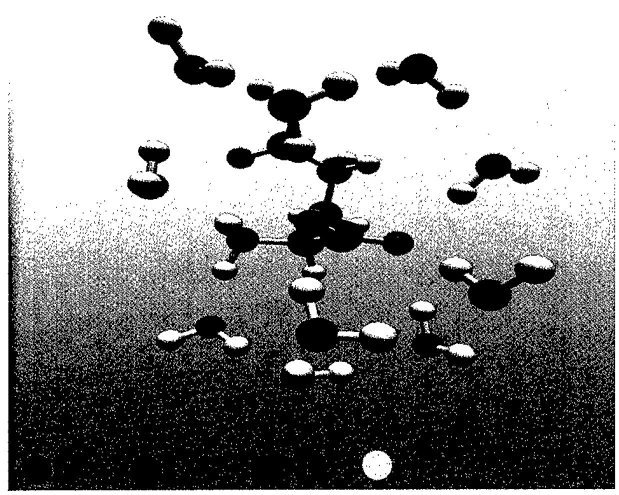
Results: The effects of solvent molecules on glutamic acid have been investigated by full ab initio calculations and the EFP approach. The results with one and two water molecules show that EFP successfully models the solvent effects on structure and energetics. In the calculations including zero, one, or two water molecules, the neutral isomer was shown to be more stable than the zwitterion. On the other hand, in the EFP calculations with 10 water molecules, where Monte Carlo methods were used to assist in finding the lowest energy configurations, the zwitterion was found to be more stable, which is the expected aqueous phase result. EFPs for methanol, dichloromethane, and chloroform have been developed, and calculations with these new EFPs agree well with full ab initio calculations. These basic developments provide an understanding for the efficient design of laser-hardened materials.

Significance: The inclusion of microsolvation and bulk solvation using the parallel routines for the EFP and self-consistent reaction field approaches within GAMESS allows a realistic prediction of properties for new materials design. Indeed, this study offers an important step toward the derivation of a general modeling approach to be used in molecular design studies of materials of interest to the DoD.

JWCO: Electronic Combat



(a)



(b)

Optimized geometry of (a) neutral and (b) zwitterionic glutamic acid including a solvation shell of 10 water molecules, from a Monte Carlo optimized starting structure

Prototype Nanoscale Electronics: Atomic Wire Arrays

S.C. Erwin, A.A. Baski, and L.J. Whitman
Naval Research Laboratory, Washington, DC

HPC Computer Resource: IBM SP [ASC MSRC]

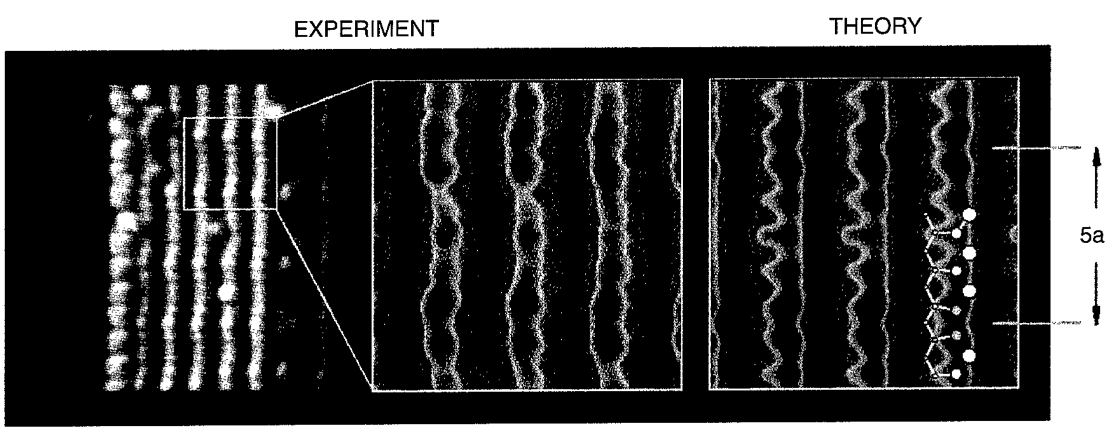
Research Objective: To elucidate the precise atomic structure—and, more importantly, the physical principles giving rise to it—of a self-assembled atomic-wire array formed when gallium is deposited on a specialized silicon substrate, Si(112). This work solved a 15-year-old question: what causes the periodic defects in the atomic wires in which every fifth or sixth gallium atom is missing?

Methodology: The calculations use state-of-the-art density-functional theory, which is the computational foundation for the modern theory of materials—including surfaces. The experiments use scanning tunneling microscopy (STM), a technique that produces images of a surface in which atomic-scale features can be clearly resolved. Used in conjunction, the interplay of these two complementary methods provides a uniquely powerful scientific tool for investigating the atomic-level structure of solid surfaces.

Results: Theoretical study demonstrates an extraordinary feature of the gallium wire arrays (which are oriented vertically in the figure panels). Through high-precision calculations of the surface energy, we have shown that the periodic defects (visible in the left panel as slightly raised bumps) cannot be eliminated by using cleaner substrates or improved procedures because they are the equilibrium—i.e., minimum energy—configuration for gallium on silicon. Rather than presenting a problem, this opens the door to nanoelectronic device applications; our calculations show that the equilibrium defect spacing can be tailored by using silicon/germanium alloys or by wafer bending. This is expected to lead to an electrically conducting surface in which the conductivity can be varied over a wide range.

Significance: At present, all microelectronics are grown on flat semiconductor surfaces, using lithographic methods that may not be scalable to the nanoscale regime. The most promising path to fabricating nanoelectronics is self-assembly of adsorbate atoms on "designer" substrates. Our work has opened the door to fabricating a very primitive prototype nanoscale device: a highly directional array of atomic wires with variable conductivity.

JWCO: Electronic Combat



STM images of single-atom-wide gallium wires (oriented vertically) on a silicon substrate. The color panels show a region containing naturally occurring defects, in which every fifth gallium atom is missing. The striking agreement between the experimental and theoretically simulated images confirms the atomic model shown in the right-hand panel.

Cooper Pairs and Phase Coherence

D.W. Hess
Naval Research Laboratory, Washington, DC
J.J. Deisz and J.W. Serene
Georgetown University, Washington, DC

HPC Computer Resource: TMC CM-500e [NRL DC]

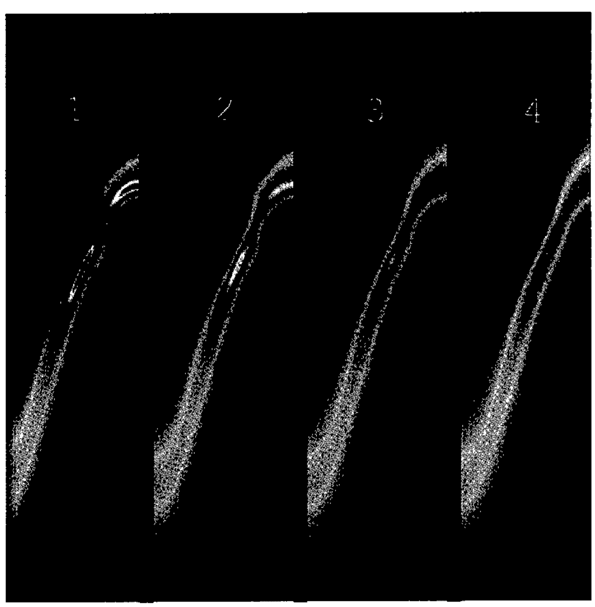
Research Objective: Photoemission experiments on the high-temperature superconductor Bi2212, and NMR and specific heat experiments on underdoped YBCO, show that electronic excitations at low-energy are suppressed above the superconducting transition temperature. A proposed explanation for this pseudogap is that as the temperature is lowered, Cooper pairs form, but fluctuations forestall the appearance of phase coherence. Phase coherence leads to macroscopic phenomena identified with superconductivity. This work uses a quantum mechanical model for interacting electrons to explore the effect of phase fluctuations on the electronic excitation spectrum as a function of temperature.

Methodology: A 2-D Hubbard Hamiltonian with an attractive interaction, together with the fluctuation exchange approximation, provides a model superconductor that includes contributions from fluctuations not contained in the standard theory of superconductivity. Calculations were performed for temperatures down to 87 K.

Results: Superconductivity was detected by calculating the internal energy and free energy in an applied magnetic field; this marks the first fully self-consistent determination of a phase transition in a conserving approximation beyond mean-field theory. The figure shows "snapshots" of the electronic excitation spectrum as the temperature is lowered through the superconducting transition. A signature of superconductivity appears only for the lowest-temperature; an evolving gap between the two red and yellow regions is evident in the left-most panel. Suppressed spectral weight is also evident in the same energy region above the transition temperature, supporting the proposal that fluctuations associated with superconductivity can lead to a suppression of spectral weight above the transition.

Significance: This work aims at a better understanding of the phenomenon of high-temperature superconductivity, of the role of fluctuations in superconductors and superconducting nanostructures, and of low-energy excitations in materials. The ability to describe these is essential for the interpretation of experiments, for exploiting novel electronic states for device applications, and for exploring and developing new device technologies both for commercial use and in support of the Navy's mission.

JWCO: Information Superiority, Electronic Combat



The electronic excitation spectrum along the (1,0) direction for four temperatures. Momentum is on the horizontal axis and energy is along the vertical axis. Color is a measure of spectral weight from red (highest) to darkest blue (lowest). Only for the lowest temperature (left-most panel) is there a signature of superconductivity. A pseudogap in the excitation spectrum is also evident separating the two red regions. Evidence of the pseudogap is also apparent in the three higher temperature panels.

Soliton Dynamics in Conducting Polymers

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University of Alabama, Birmingham, AL
A.T. Yeates
U.S. Air Force Academy, Colorado Springs, CO
D. Dudis
Air Force Research Laboratory, Wright-Patterson AFB, OH
J.H. Weare
University of California San Diego, La Jolla, CA

HPC Computer Resource: TMC CM-5E [NRL DC] and TMC CM-5 [AHPCRC DC]

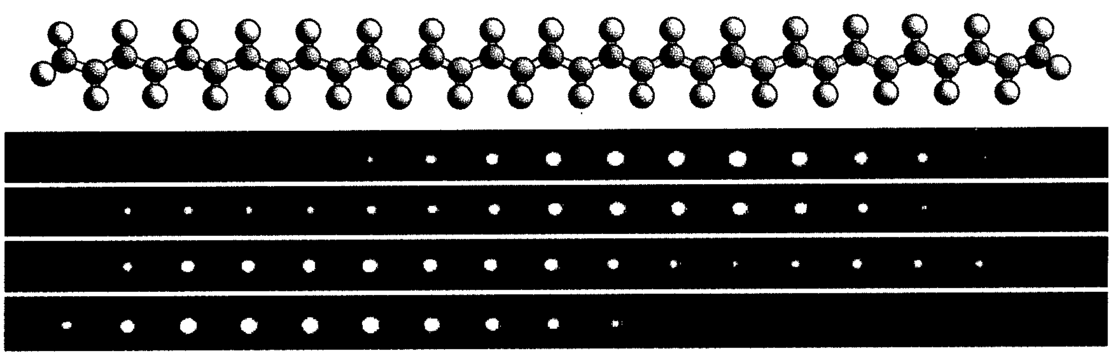
Research Objective: To reliably predict chemical and physical properties of conjugated polymers, which provide a new class of conducting and optical materials, and to design new electronic and optical materials based on these molecules. To achieve these goals, it is necessary to develop new, highly efficient first-principles calculation codes for massively parallel computers and networks of workstations.

Methodology: The atomic geometry and electronic properties are computed using local spin density function methods. In order to capture properties of the delocalized conduction electrons, a planewave basis set is used. For large systems, more than 100,000 basis functions per orbital are needed. However, the cost of this large number of basis functions is offset by high parallelism of the algorithms. Our new parallel ab initio molecular dynamics (PAIMD) simulation code allows us to simulate dynamics of large polymer systems from first principles efficiently on the TMC CM-5.

Results: Soliton dynamics plays a dominant role in certain types of conjugated polymers. We have directly simulated dynamics of soliton with quantum chemical accuracy and obtained the size of a traveling soliton, activation energy, mobility, effective mass, and other dynamical properties.

Significance: Static structures of solitons have been investigated with conventional quantum chemistry methods. However, its dynamical properties have not been investigated at ab initio levels due to the lack of an efficient computational method and sufficient CPU power. Therefore, dynamical properties essential to the electric conduction were not well understood. Using our PAIMD, we are able to determine them with the same accuracy as the conventional static quantum chemical calculations.

JWCO: Information Superiority



Motion of spin polarization associated with a neutral soliton in polyacetylene. Spin polarization is localized on every other carbon atom and travels from right to left.

Computational Alloy Design of High-Temperature Structural Intermetallics

C. Woodward and S.A. Kajihara
UES Inc., Dayton, OH
D.M. Dimiduk
Air Force Research Laboratory, Wright-Patterson AFB, OH

HPC Computer Resource: Cray C916 [ASC and CEWES MSRCs]

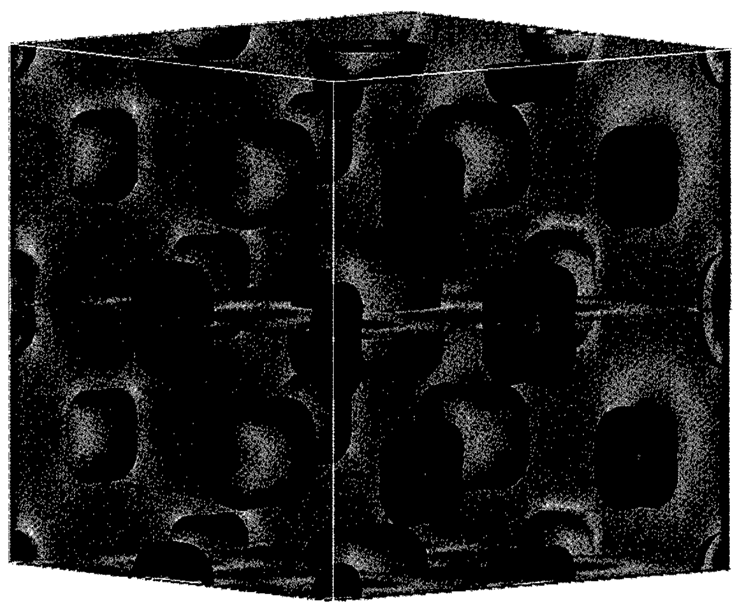
Research Objective: To provide a computational tool for screening the effects of solid solutions on the flow and fracture properties of high-temperature structural intermetallics. A nanoscale, quantum mechanical model is used to describe the response of a host material to changes in alloy chemistry for structural materials (TiAl and NiAl) that are of interest to the Air Force. The goal is to improve the strength and creep properties of materials used in aerospace and domestic applications, such as high-performance turbine engines, rocket engines, and Earth-based power generation.

Methodology: A state-of-the-art quantum-lattice dynamics code based on the density functional method is used to determine the electronic structure and the atomistic response of a host lattice to substitutional point defects. The point defect energies are calculated to high precision, and changes in the elastic moduli are calculated using a local stress-tensor method.

Results: HPC resources were used to study 14 defects centers in γTiAl, including Si, Nb, Mo, W, and Ta as solid solutions. Defect energies calculated using first-principles methods are used in a thermodynamic model to find the density of constitutional and thermal defects. This yields the site preferences of the solid solutions and the vacancy concentration as a function of composition and temperature. The response of the lattice to the solute atoms, the lattice relaxation, and the changes in the local interatomic forces are used in continuum models to determine the effects these solutes have on the mobility of active deformation modes. From these calculations, we can predict changes in strength as a function of temperature and composition.

Significance: Solid solutions are often used by alloy designers to modify the intrinsic flow and fracture of intermetallic alloys. Typically, extensive screening studies are required to determine the influence of various solid solutions on plastic deformation of the host material. These computational methods offer a tool for alloy designers to determine favorable alloy compositions. For example, the electronic structure results determine which compositions minimize the concentration of thermal vacancies, and it is at these compositions that diffusional creep mechanisms will be suppressed. Also, the predicted solute-dislocation interaction parameters can be used to predict the optimum composition for low-temperature yielding and high-temperature strength. This work has identified two ternary alloys that are expected to have improved flow and fracture properties.

JWCO: Precision Force



Charge density iso-surface of Ta solute atom in γTiAl

Design of New POSS Species

M.S. Gordon and T. Kudo
Iowa State University, Ames, IA

HPC Computer Resource: IBM SP [MHPCC DC] and Cray C90 [ASC MSRC]

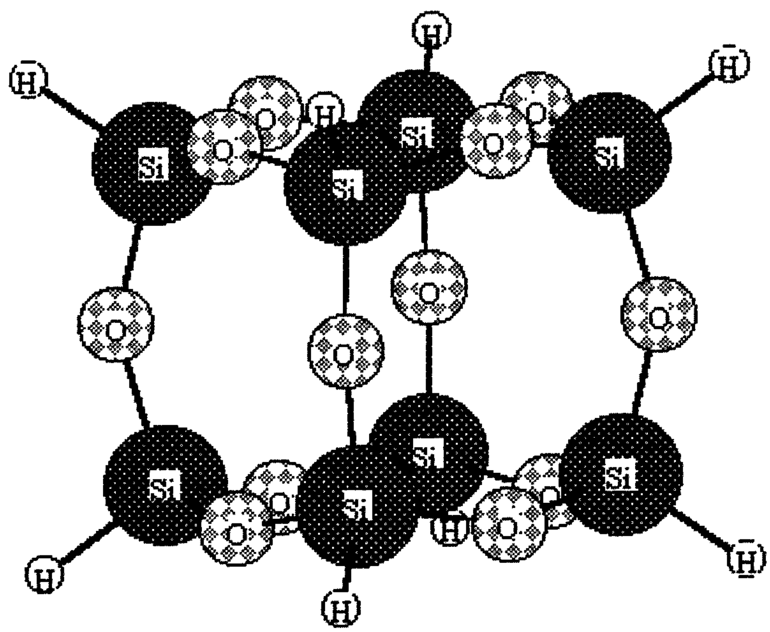
Research Objective: To use computational chemistry to determine plausible routes to the polyhedral oligomeric silsesquioxanes (POSS) and then to propose new synthetic routes and new species.

Methodology: POSS hold great promise as lubricants and protective coatings for space vehicles, among many other uses. At present, however, little is known about the mechanism of formation of these species or about the role of solvent, catalysts, or pendant chemical groups. High-level ab initio methods, including the incorporation of electron correlation effects, are used to determine the molecular and electronic structures of POSS precursors, as well as the transition states and associated barrier heights leading to POSS. The quantum chemistry codes GAMESS and GAUSSIAN have been used to perform the calculations. The parallel features of GAMESS have been essential for the success of this project.

Results: The mechanism for the hydrolysis of the starting material $RSiCl_3$ to trihydroxysilane $RSi(OH)_3$ is predicted to occur in three steps, each step corresponding to the elimination of HC_1 and incorporation of an OH group. The subsequent condensation of two $RSi(OH)_3$ species via elimination of a water molecule proceeds via a hydrogen-bonded intermediate structure. Most importantly, it is found that the gas phase energy barriers for these reactions (both hydrolysis and condensation) are high (20-30 kcal/mol at the highest levels of theory) but that the barrier heights are reduced dramatically (to 0-5 kcal/mol) when one extra water molecule is added. This provides strong evidence of the importance of solvent effects on the mechanism for POSS formation. Further investigations of the solvent effects, as well as studies of the effects of various catalysts, are under way.

Significance: A fundamental understanding of the mechanism of formation of POSS-related systems is a critical step in controlling the synthesis to produce specific compounds for DoD-relevant applications. These studies show the importance of solvent effects in the mechanism of POSS formation.

JWCO: Joint Readiness and Logistics



Optimized geometry of the parent POSS compound, $Si_8O_{12}H_8$

Modeling Contaminant Chemistry in the Environment

J.D. Kubicki and S.E. Apitz
Space and Naval Warfare Systems Center, San Diego, CA

HPC Computer Resource: Convex Exemplar SPP 1000 [SSCSD DC] and Cray C90 [ASC MSRC]

Research Objective: To answer basic research questions involved with reducing costs in the management of contaminated sediments. Molecular modeling of organic contaminants in the environment is being used. Knowledge of chemical interactions between organic contaminants and sediments leads to increased understanding of the risk and fate associated with petroleum products released near naval shipyards.

Methodology: This study was designed to examine polycyclic aromatic hydrocarbon (PAH) adsorption to minerals and to test whether chemical interactions of PAHs in the environment could affect a quantitative structure-activity relationship (QSAR) that has been shown to be a good indicator of phototoxicity. Minimum energy structures were determined with PM3 methods using the program HyperChem 5.0 and with HF/3-21G** and Becke3LYP/6-31G* basis sets using Gaussian 94.

Results: To predict the effects of adsorption on chemical stabilities and toxicities of PAHs, three benzene-$[Al(OH)_{3+x}]^{3-x}$ dimers were energy-minimized with the HF/3-21G** and B3LYP/6-31G* basis sets. Naphthalene, pyrene, and dibenzo[*b,i*]anthracene were modeled with an Al-hydroxide surface cluster, $Al_9O_{34}H_{41}$, with PM3 semi-empirical quantum mechanical calculations. In some cases, such as the benzene-$[Al(OH)_2(OH_2)]^+$ dimer calculations with HF/3-21G** and B3LYP/6-31G*, the changes in the chemical stability can be on the order of 10%. Thus, significant shifts in molecular stability could occur with adsorption. However, these shifts decrease the chemical stability with regard to degradation. If this is the case for adsorbed benzene and PAHs, then these organic contaminants would be more susceptible to degradation in the adsorbed state rather than more resistant to degradation, which is what is commonly observed.

Significance: Although fairly strong interactions can occur between PAHs and a mineral surface, the chemical bonding is not strong enough to significantly change the chemical stability and toxicity of the contaminants. Furthermore, bonding energetics between organic contaminants and mineral surfaces are an order of magnitude weaker than the bonding between natural organic matter and mineral surfaces. Thus, organic contaminants will not interact directly with mineral surfaces if natural organic matter is already present. These models suggest that decreased biodegradability of organic contaminants is due to a physical sequestration phenomenon within the sediment matrix. Hence, the environmental risk associated with sediments contaminated by PAHs is lower than would be predicted by models. Consequently, cleanup standards for contaminated sediments could be set higher in some instances, which would decrease the volume of sediments requiring remediation and result in significant cost savings.

JWCO: Chemical/Biological Warfare Defense and Protection

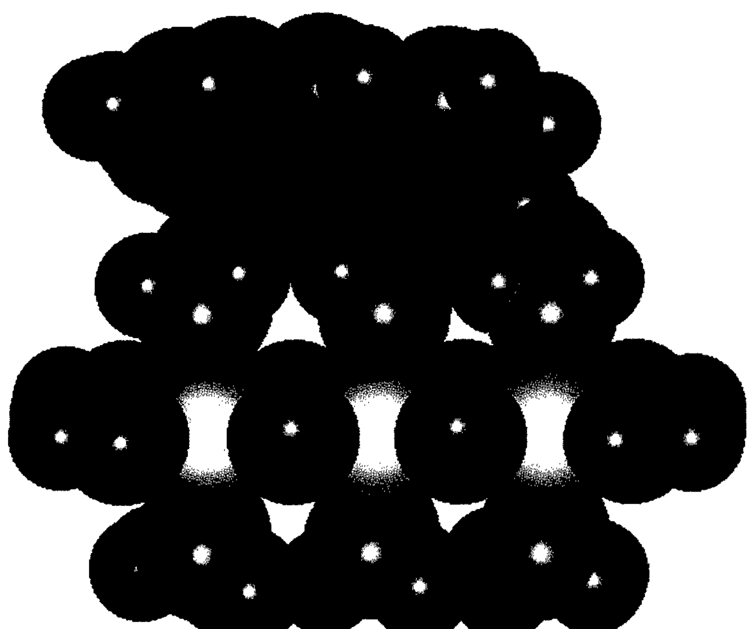


Image of pyrene, an organic contaminant found in petroleum products, adsorbed onto an aluminum hydroxide mineral surface as modeled with quantum mechanics calculations (blue: carbon; red: hydrogen; green: oxygen; yellow: aluminum). Computations like this increase our understanding of the bioavailability and fate of organic contaminants in marine sediments with the goal of decreasing costs in the management of contaminated sediments.

Quantum Chemical Modeling of the Atmospheric Destruction of the Nerve Agent Sarin (GB)

S.W. Bunte, C.F. Chabalowski, and B.M. Rice
Army Research Laboratory, Aberdeen Proving Ground, MD

HPC Computer Resource: SGI PCA [ARL MSRC]

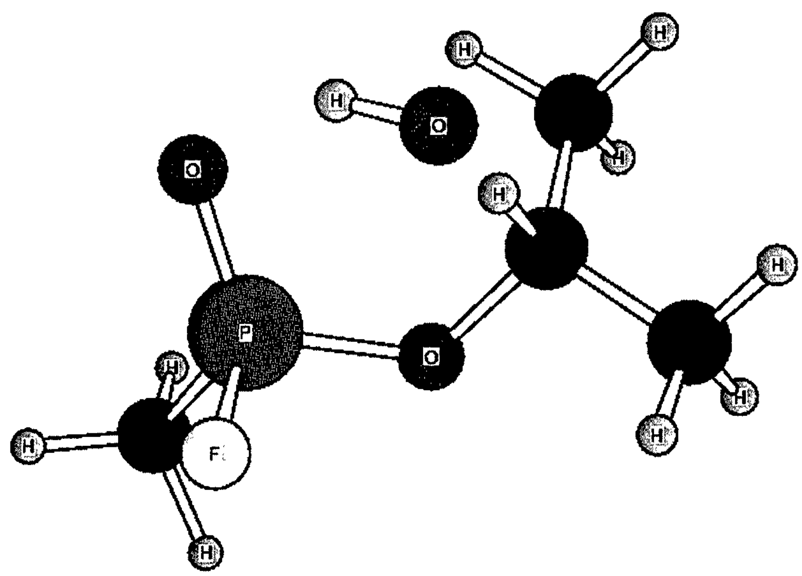
Research Objective: To characterize the potential energy surfaces of chemical reactions leading to the atmospheric destruction of the chemical agent sarin (GB). Additionally, spectral signatures of GB and its reaction intermediates are investigated to facilitate detection of GB in the atmosphere.

Methodology: Quantum mechanical calculations at the density functional theory and MP2 levels were used to characterize the potential energy surfaces of chemical reactions leading to the atmospheric destruction of the chemical agent sarin. Additionally, predictions of the infrared spectra of GB and the intermediate stable species along the reaction pathways have been determined.

Results: The first reaction studied involves the abstraction of the tertiary hydrogen by OH radical attack. This reaction, which results in the formation of a GB radical species, is essentially spontaneous because the activation barrier is less than 1 kcal/mol. The decomposition of the GB radical has also been studied. The barrier to further decomposition is 24.5 kcal/mol, which is of sufficient height to prevent this reaction from occurring under atmospheric conditions. This suggests that the radical is long lived and will react with other atmospheric species.

Significance: There has been a renewed interest in understanding the chemistry of nerve agents as an aid in the destruction of the nation's chemical weapon stockpile. This study provides mechanisms for the degradation of the chemical agent GB and spectral signatures of the intermediate and final stable products that can be used to detect and identify the presence of GB in the atmosphere.

JWCO: Chemical/Biological Warfare Defense and Protection



MP2 optimized structure of the GB + OH transition state

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Cooper Pairs and Phase Coherence

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Modeling Contaminant Chemistry in the Environment

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Computational Electromagnetics and Acoustics

Computational Electromagnetics and Acoustics is a seamless interdisciplinary modeling and simulation technology for communication, surveillance, detection, and precision strike. This critical computational technology is based on mathematical descriptions of electromagnetic and acoustic phenomena that involve wave generation, propagation, diffraction, and refraction. A primary objective of CEA is to develop scalable, high performance numerical procedures to meet weapons system design and modification as well as operational needs. Accomplishments in CEA cover a dynamic range from automatic target recognition for combat operations to solid scientific advancements that will lead to battlefield dominance. Specifically, an efficient numerical procedure has been verified in generating synthetic aperture radar imagery for complex targets that are embedded in realistic scenes. Significant progress in innovative hybrid CEA techniques for mission planning and antenna and microcircuit design was also made for full sensor analysis over a wide range of operating frequencies. Solid accomplishments were also attained in the area of full-scale electromagnetic scattering simulation for jet engines. For the first time, accurate modeling of fine blade features are realizable to overcome a long-lasting shortfall of accurate modeling requirements. The successes of CEA on the more fundamental scientific level can be summarized in impressive computational efficiency improvement, novel ideas of high-resolution numerical algorithm developments, and efficient calculation procedures. All of these improvements to knowledge have permitted simulations of unprecedented complexity and dimensions of scatterer. The advancements based on concepts of domain fusion have extended the frequency spectrum and improved predictive accuracy for both electromagnetic and acoustic applications.

Joseph J.S. Shang
Air Force Research Laboratory
Wright-Patterson AFB, OH
CTA Leader for CEA

Automatic Target Recognition and Scene Generation Code

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HPC Computer Resource: Intel Paragon [AFRL/ID DC] and IBM SP [ASC MSRC and MHPCC DC]

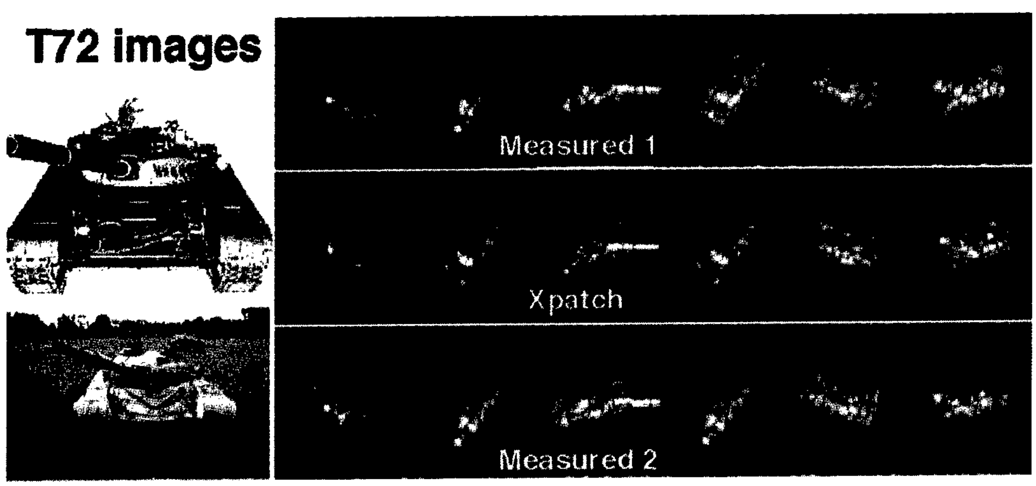
Research Objective: Automatic target recognition (ATR) system development and testing often requires the generation of synthetic aperture radar (SAR) imagery for complex targets embedded in realistic scenes at X-band. The only cost-effective way to produce the copious amounts of SAR imagery required is via computational electromagnetic techniques. The maturation of asymptotic methods under this effort for massively parallel computers is critically needed to fulfill the data requirements for ATR, low-observable system design, and endgame modeling and simulation at frequencies of L-band and above.

Methodology: Many improvements in high-frequency codes still need to be made, including higher order diffractions, creeping waves, traveling waves, and complex materials. Many of these improvements are planned to be implemented in Xpatch. They include new incremental length diffraction coefficients and geodesic ray tracers to predict creeping waves on complex objects, new asymptotic methods for cavities developed under the noncooperative target identification (NCTI) engine project, and further parallelization enhancements for portability between HPC sites.

Results: The figure shows a T72 tank used for field measurement by X-band radar, a display of the CAD model used by Xpatch, and three sets of SAR images—two by measurements and one by Xpatch. Such good correlation between measured and computed SAR images is unprecedented. Xpatch generates results like these for the ATR community on a daily basis.

Significance: The asymptotic prediction code Xpatch has been widely accepted across DoD as the best high-frequency radar signature prediction code for realistic targets. It is being used to populate the first operational databases for NCTI and is also the basis for the DARPA moving and stationary target acquisition recognition (MSTAR) real-time target chip generation system. The databases being generated with Xpatch are the first-ever utilization of predictions for operational systems.

JWCO: Combat Identification



SAR images of T72 tank: comparing two sets of measurements taken by an airplane and Xpatch computation. The frequency is X-band and the resolution is 12 inches.

Synthetic Sensor Phenomenology for Fusion

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HPC Computer Resource: IBM SP and SGI Origin 2000 [ASC MSRC] and Intel Paragon [AFRL/ID DC]

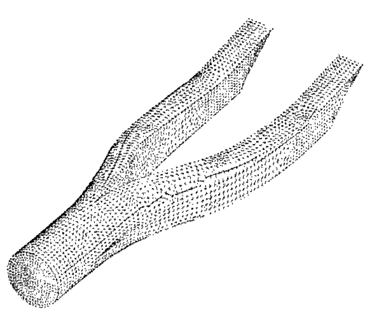
Research Objective: To develop a scalable software suite for hybrid computational electromagnetics (CEM) in support of radar analysis, antenna design, circuit design, electromagnetic interference/electromagnetic capability, mission planning and effectiveness studies, and for critical real-time modeling and simulation in multiple DoD and commercial applications. This project includes the integration of low- and high-frequency codes to form a hybrid prediction approach that will extend the frequency range and accuracy of existing prediction technologies to support full sensor analysis over a wide range of operating frequencies.

Methodology: A hybrid code is being developed based on the hand-off approach for scattering and radiation by large complex targets with indentations such as cavities, microstrip antennas, gaps, cracks, and slotted arrays. Dominant interaction between indentations and their host platform is accounted for by "impedance" matrices and the reciprocity theorem. Component codes to be integrated into this hybrid are Xpatch, SWITCH, UPRCS, FISC, Xbrick, XSlot, and XCavity. The hand-off approach will be extended in the hybrid code to protruding scatterers such as fins and wings on an airplane. By using low-frequency codes, such as FISC, SWITCH, or UPRCS, the protruding scatterer will be characterized by equivalent electric and magnetic currents represented in matrix form. The resultant matrix will be read into Xpatch for interaction computation between protruding scatterers and the host platform. The jet engine scattering code AIMJET will be enhanced by incorporating engine periodicity and modal matrix sparsity, using a periodic Green's function, implementing a memory reduction scheme, and parallelizing the code. AIMJET will also be integrated with Xpatch through incorporation into the SWITCH code.

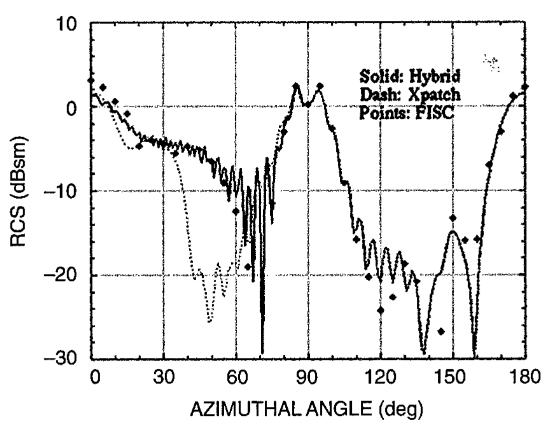
Results: Successful hybridization has been implemented for a range of problems, including the presence of cracks, gaps, cavities, patch antennas, and slotted waveguide arrays located on complex targets such as aircraft. The figures demonstrate the hybridization of high- and low-frequency codes to solve engine inlet types of problems, such as the VFY218 inlet and the C29 aircraft inlet. Validation includes comparison to measurements and full-wave, nonhybrid, numerical electromagnetic techniques.

Significance: The hybrid prediction codes being developed under this area are the next major step in improving the accuracy of computational electromagnetic prediction codes. With these codes, it will be possible to predict the accurate solution for an aircraft engine cavity—the most dominant and complex scattering mechanism on complex air vehicles that has perplexed the CEM community for many years.

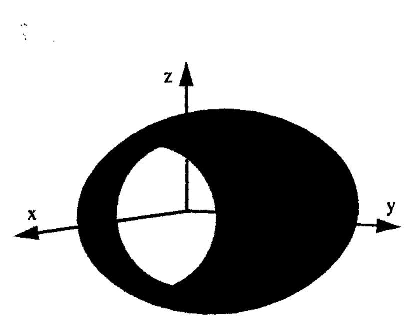
JWCO: Combat Identification



VFY218 inlet



Computed monostatic radar cross section at 2 GHz, EL=0, HH pol



C29 inlet example (no blades)

Electromagnetic Scattering from Complex Geometries

Capt. D.C. Blake, U.S. Air Force, J.S. Shang, and H.J. Thornburg
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HPC Computer Resource: SGI Origin 2000 [ASC MSRC]

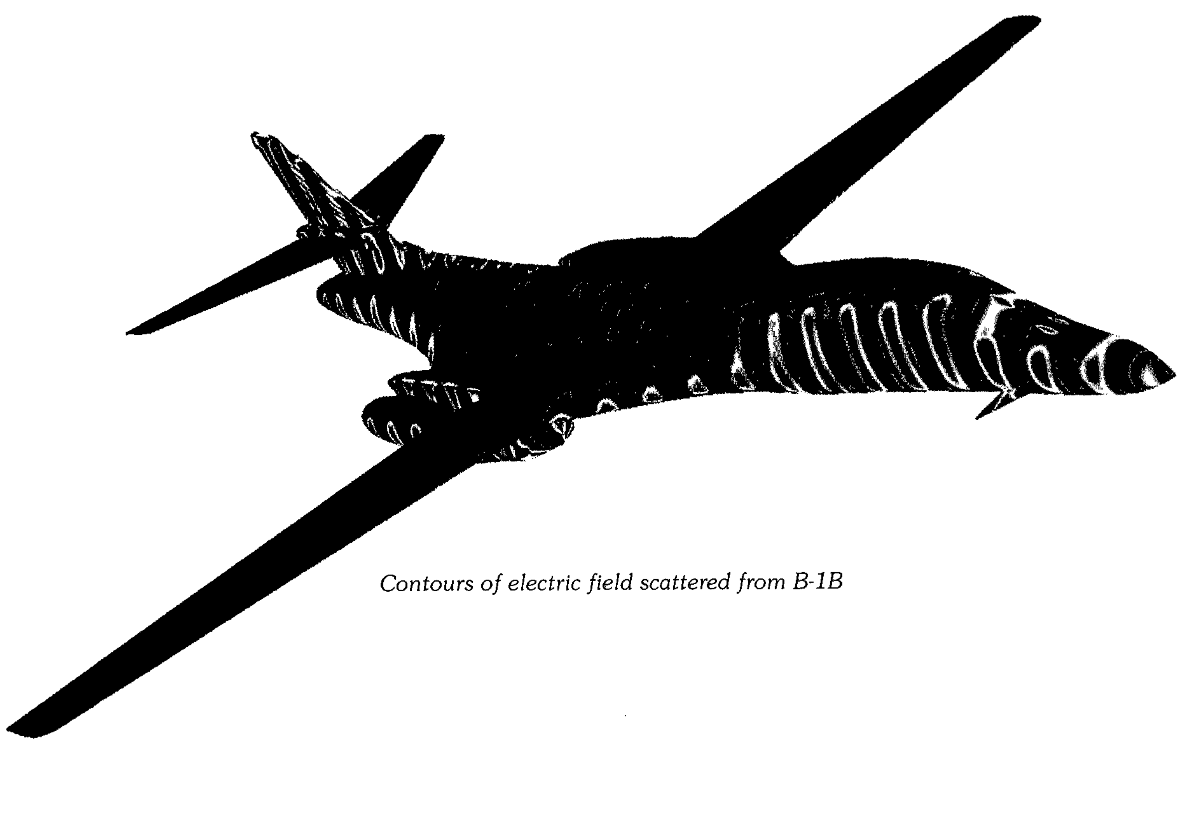
Research Objective: To develop the tools and techniques necessary to numerically simulate electromagnetic wave scattering from extremely large and complex objects.

Methodology: A finite-volume time-domain (FVTD) algorithm is used to solve the Maxwell equations in regions on and around highly complex geometries. These regions can be gridded using any combination of structured multizone or overset grids. Emphasis is placed on generality and flexibility so that a wide range of geometrical configurations can be examined with few if any computer code modifications.

Results: The computer code developed as part of this effort has proven to be highly versatile. Electromagnetic scattering simulations have been successfully conducted on a variety of complex configurations ranging from finned missiles to full-scale aircraft. The most demanding simulation thus far performed involves the B-1B, which was gridded using two multizone grids consisting of approximately 28.5 million grid points and 700 grid blocks. Certain regions of the multizone grids overlap, and in those regions, information is exchanged between the grids via interpolation. Despite the complexity of this configuration, calculations using between 32 and 64 processors of the SGI Origin 2000 were begun within hours after grid generation was completed.

Significance: The capability to accurately and efficiently simulate the physics of electromagnetic wave propagation is essential to the design process of future generation weapons systems. As a result of this effort, simulation turnaround times have been reduced from months to days. This represents a significant stride toward highly accurate assessments of full-aircraft stealth characteristics during the design cycle.

JWCO: Electronic Combat, Combat Identification



Contours of electric field scattered from B-1B

Electronic Fields and Surface Current Simulations for Jet Engine Nozzles

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HPC Computer Resource: Intel Paragon [ASC MSRC]

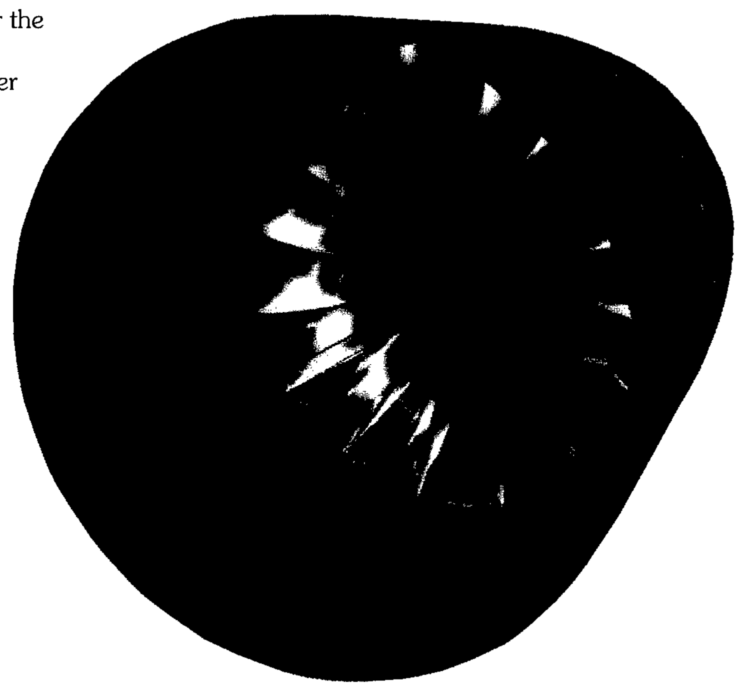
Research Objective: To develop and demonstrate the capability of full-scale electromagnetic scattering calculations for jet engine nozzles and in particular, to demonstrate the scalability of method-of-moment (MoM) based CARLOS codes in the full-scale simulation of jet engines for warfighters.

Methodology: In these simulations, the electromagnetic interactions were formulated in terms of discretized integral equations solved by the MoM (Galerkin) procedure. The GE404 jet engine nozzle was run both with and without *n*-fold rotational symmetry, with an *n*-fold partitioned matrix equation. An untreated GE404 engine nozzle with 16 blades was simulated with 14,272 faceted unknowns; the treated nozzle was simulated with 28,544 faceted unknowns. The Boeing SLIC advanced solver was used in the simulations. SLIC is able to run on processors of unequal capability with an arbitrary number of nodes with a ProSolver 2.0 interface. The solver is implemented with a message-passing interface version of an out-of-core solver implemented for either a loosely coupled cluster of workstations or a tightly coupled supercomputer.

Results: The untreated and treated nozzles were run on a Silicon Graphics workstation. Results were also obtained using the Paragon supercomputer with 196 multiprocessing compute nodes having 64 Mbytes of memory on each node. For the radar cross-section calculations, two polarizations for 181 illumination angles were computed. The figure shows representative results of these simulations depicting current images. Using the *n*-fold rotational symmetry option in CARLOS, both the untreated and treated cases were run with 872 and 1,748 unknowns respectively.

Significance: The efficacy of the CARLOS family of codes on a massively parallel computer has been demonstrated for the simulation of complex engine inlet configurations. In particular, the flexibility and efficiency of the SLIC solver has been demonstrated, as well as the new *n*-fold rotational symmetry feature of CARLOS. Boeing's experience shows that use of the rotational symmetry feature in conjunction with the massively parallel processing environment can provide a dramatic increase in the size of problems possible for electromagnetic computations and simulations.

JWCO: Joint Theater Missile Defense, Joint Readiness, Electronic Combat, Information Warfare



Current image on GE404 nozzle (2 GHz, vertical polarization)

Jet Engine Scattering Using Fast Integral Methods

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K.C. Hill
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HPC Computer Resource: Cray C90 [ASC MSRC]

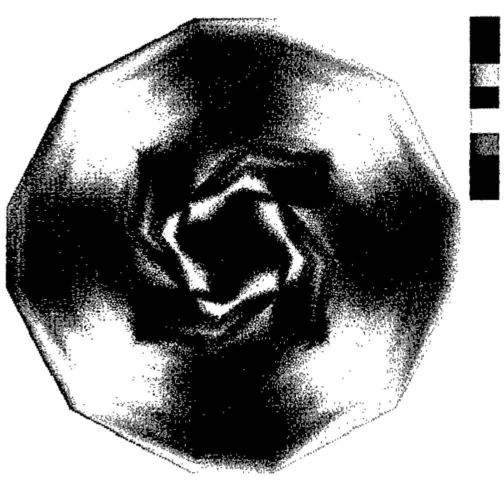
Research Objective: To develop an efficient numerical method to achieve full-scale characterization of jet engine scattering for realistic in-flight (dynamic) simulations.

Methodology: Jet engine characterizations present us with unique challenges because of their large size coupled with the need for an accurate modeling of the fine blade features and multiple engine stages. Also, actual flight computations require rotating blade simulations that involve numerous repeated calculations that must normally be performed independently. Without any optimization, a simulation of a real size is beyond our computational capability. Over the past two years, we devised a methodology that takes advantage of blade periodicity to reduce the problem domain down to a single slice. Specialized matrix compression techniques based on the adaptive integral method (AIM) were used to further reduce the CPU requirements to O(N1.5) from O(N2). An important outcome of our research is the extraction of dynamic effects as a postprocessing step, thus avoiding a need for recomputation.

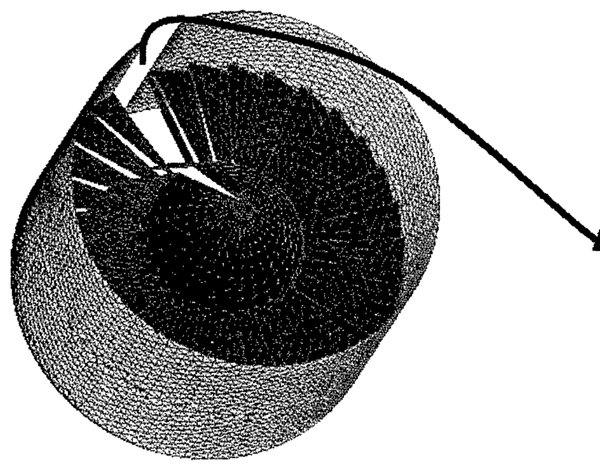
Results: Our exploitation of blade periodicity, matrix compression schemes used, and parallelization allowed us to reduce the CPU time for an entire engine characterization to within 4 to 7 hours on a C90 platform, a four order-of-magnitude improvement over previous implementations. This CPU corresponds to a full-scale fighter engine at 2 GHz. The accompanying figures show the actual C-29 engine geometry and results.

Significance: Engine scattering contributes significantly to the radar signature of an aircraft. By using AIM matrix compression, blade periodicity, and HPC computers, accurate prediction of the complex engine scattering problem is now possible. This solution will enable engine prediction to be part of the aircraft design.

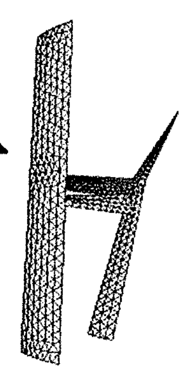
JWCO: Combat Identification, Electronic Combat



Field image at a small distance from engine



C-29 engine with one slice removed



Engine slice used for computation

Conformal Antenna System Development

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The Boeing Company - Phantom Works, St. Louis, MO

HPC Computer Resource: Intel Paragon [ASC MSRC]

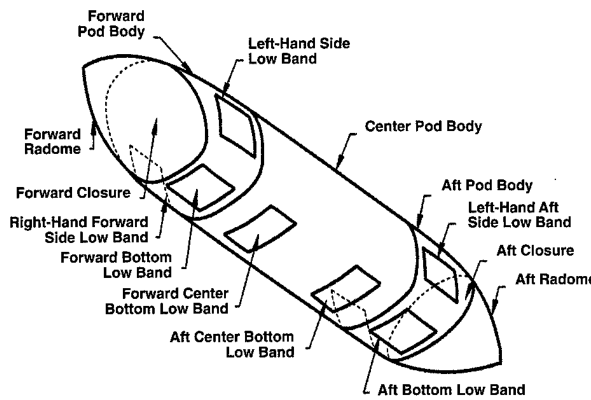
Research Objective: To demonstrate the feasibility of full-scale dynamic simulation of a complex RF/EW system for external undercarriage on a combat aircraft, such as the F-15 or F/A-18E/F, using massively parallel computers running an advanced method-of-moments (MoM) antenna code (CARLOS v.4.0).

Methodology: Because a very high degree of accuracy was required to account for the multiplicity of electromagnetic interactions (antenna coupling, element phasing, cavity treatments, feedlines, and electromagnetic interference (EMI)), a MoM formulation was used to solve Maxwell's equations in integro-differential form. The code implementation was the CARLOS antenna code, which features specialized basis functions for accurate analysis of feeds and tuning networks such as baluns. A special surfacing tool ZONI3G was used for rapid definition of the configuration and the antenna apertures. The sequence of simulations extended over a broad range of frequencies with up to 250,000 unknowns using various solver strategies.

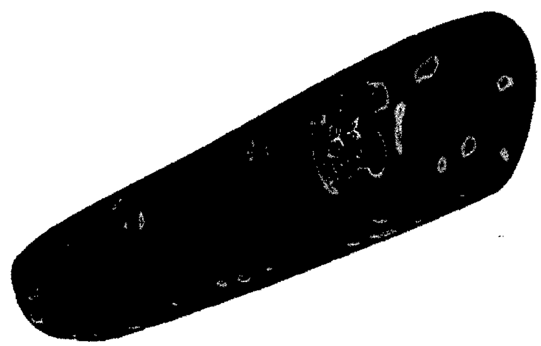
Results: The resulting system of arrays achieved full hemispherical coverage with horizontal and vertical polarization and a 3:1 bandwidth for the primary arrays. The cavities for the low-band systems used specialized anisotropic treatments requiring only a one-inch depth penetration into the pod. Numerical simulations were used to optimize shape and placement of the antenna elements to maximize electronic steerability with minimum crosscoupling and EMI.

Significance: The dynamic simulations established the proof of concept of this system. Subsequent experimental data confirmed the efficacy of these results with a minimum of range time and test fixture mockup. Overall, the time compression using this numerical prototyping approach reduced the design cycle time 10-fold and the range test expenses by at least a factor of 5. Under the sponsorship of the HPC/CHSSI program, this numerical prototyping technology is being incorporated into a new hybrid code (HYPACED), which will extend this technology for even more complex airborne systems.

JWCO: Precision Force, Combat Identification, Joint Theater Missile Defense



Antenna analysis modeling showing the final layout of arrays



Representative current distributions with active forward right-hand side low-band array

Undercarriage deployment (centerline) on F/A-18E/F

Modeling of Acoustic Scattering from Submerged Cylindrical Shells

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HPC Computer Resource: Cray T3D [NUWC DC]

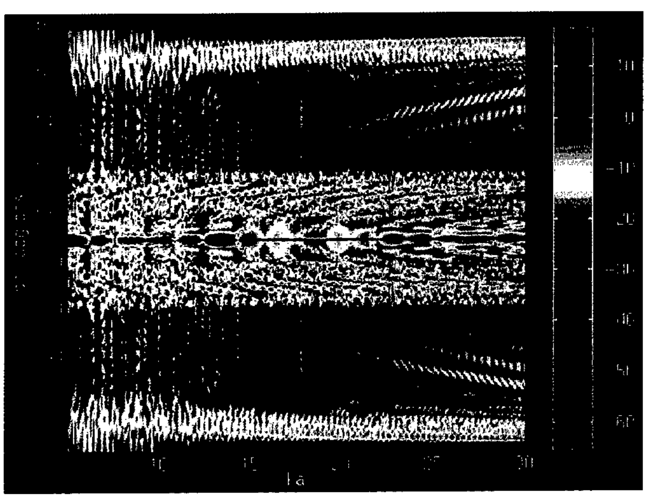
Research Objective: To construct an analytical model, valid over a broad frequency range, for acoustic scattering from a finite rib-stiffened cylindrical shell with two planar endcaps. The structure is submerged in a fluid and is subjected to an incident wave impinging on the shell from a source in an arbitrary direction.

Methodology: The current investigation uses the classical shell equations for the cylindrical part of the structure, and classical bending and plane stress equations for the endplates and stiffeners. The shell is segmented at each stiffener location. The homogeneous and particular solutions are found for each segment of the cylindrical shell and the endplates. The value of the constants associated with the homogeneous solution is found by enforcing the boundary conditions of the continuity of displacements/rotation and balance of forces/moment at each interface. The Kirchoff-Helmholtz formulation is used to determine the resultant scattered field of the structure due to an incident acoustic wave as a function of frequency and aspect angle.

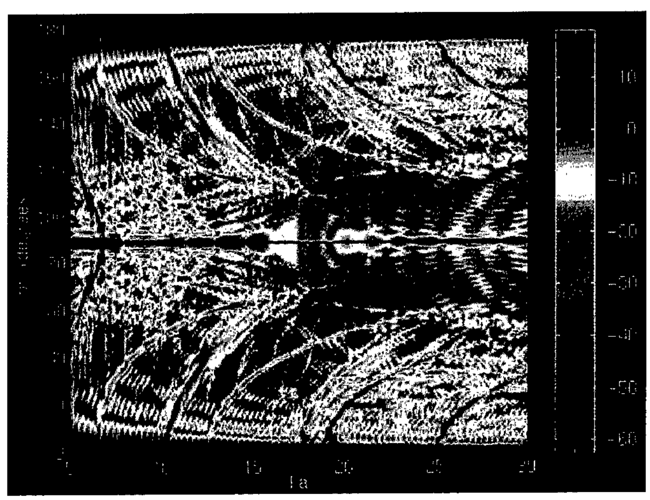
Results: Consider a cylindrical shell with length-to-radius ratio of 10 and thickness-to-radius ratio of 0.05. The shell is capped with circular endplates with thickness-to-radius ratio of 0.05. The material properties of the structure are those of steel, and the fluid properties are those of water. The left-hand figure illustrates the calculated monostatic target strength for the case of no rib stiffeners as a function of nondimensional frequency ka and aspect angle ϕ. The right-hand figure shows results for a rib-stiffened shell with stiffener-height-to-shell-radius ratio of 0.2 and spacing-to-radius ratio of 0.5.

Significance: Finite-element methods are generally limited to relatively low frequencies. This research was undertaken to provide a mathematical model that is valid over a wide frequency range and to investigate the role of stiffener and bulkhead discontinuities on scattering in a continuous manner with respect to frequency. This analysis is generic and applies to the scattering from common naval architecture such as submarines, unmanned underwater vehicles, and mines.

JWCO: Combat Identification



Farfield monostatic target strength in dB for submerged unstiffened shell with endplates



Farfield monostatic target strength in dB for submerged rib-stiffened shell with endplates

Efficiency of High-Power Microwave Source Improved Through Virtual Prototyping

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S.L. Colella and J.J. Watrous
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HPC Computer Resource: IBM SP [MHPCC DC]

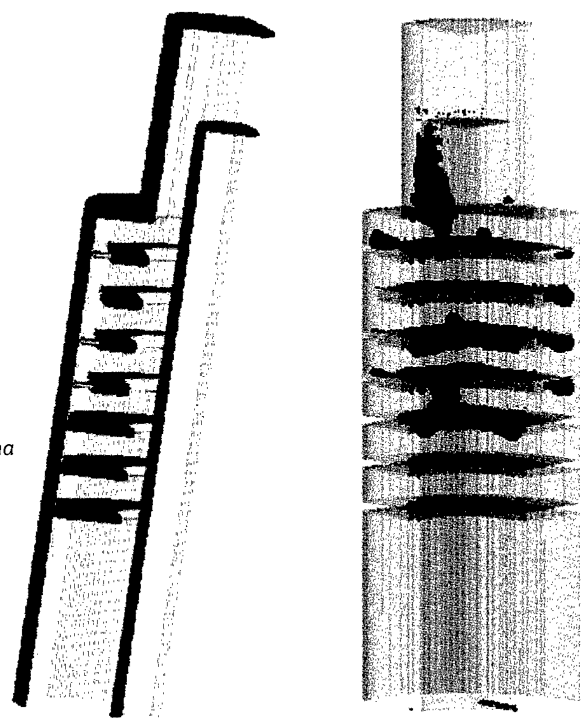
Research Objective: To apply a series of in-house research codes to the problem of virtual prototyping of high-power microwave (HPM) devices. Such virtual prototyping can be used to significantly reduce cost and development time.

Methodology: The three-dimensional particle-in-cell (PIC) code ICEPIC is a portable, scalable package that was developed to take advantage of the many parallel assets available to the DoD community. PIC codes are the tool of choice for simulation of the diode and cavity regions of HPM sources. ICEPIC was one of the first fully functioning PIC codes to be implemented on a parallel platform.

Results: The future warfighter may use HPM weapons to gain a significant advantage in electronic combat. HPM weapons may be used to disrupt or damage electronic systems, disabling enemy defenses and weaponry. Collateral damage is also reduced with such devices, allowing the warfighter to strike with precision force. Development of the sources for such devices is challenging because very high powers and small lightweight packages are required. The ICEPIC code can be used for fine-tuning well-understood devices and for testing radical new designs. One measure of a source's performance that is of great importance is the efficiency (power emitted divided by power supplied). Higher source efficiency means that more power can be delivered to a target with a smaller source and less stored energy. MILO is a relatively new source that has been developed as a possible candidate for use in HPM weapons. The inductively coupled MILO is the result of a number of simulations performed to explore new designs to improve efficiency. This device was found to achieve higher efficiency, smaller design, and a faster growth rate by coupling of the magnetic field through slots cut in the outer portion of the radial vanes.

Significance: To meet the strict demands in performance and delivery of an HPM weapon, a high efficiency is required. Designs such as the inductively coupled MILO shown below may be sufficient to meet these demands. A new design of an HPM source with significant differences from existing devices can be thoroughly investigated in two to six work-months using existing software and computational resources, as demonstrated here. This is significantly faster and cheaper than a comparable experimental effort.

JWCO: Precision Force, Electronic Combat



Quarter slice of an inductively coupled MILO (left) and the extrema of the electric (red) and magnetic (green) fields in the device (right)

Can Controlled Explosions Be Used to Amplify Magnetic Fields to Power Advanced Weapons?

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NumerEx, Albuquerque, NM

HPC Computer Resource: IBM SP [MHPCC DC]

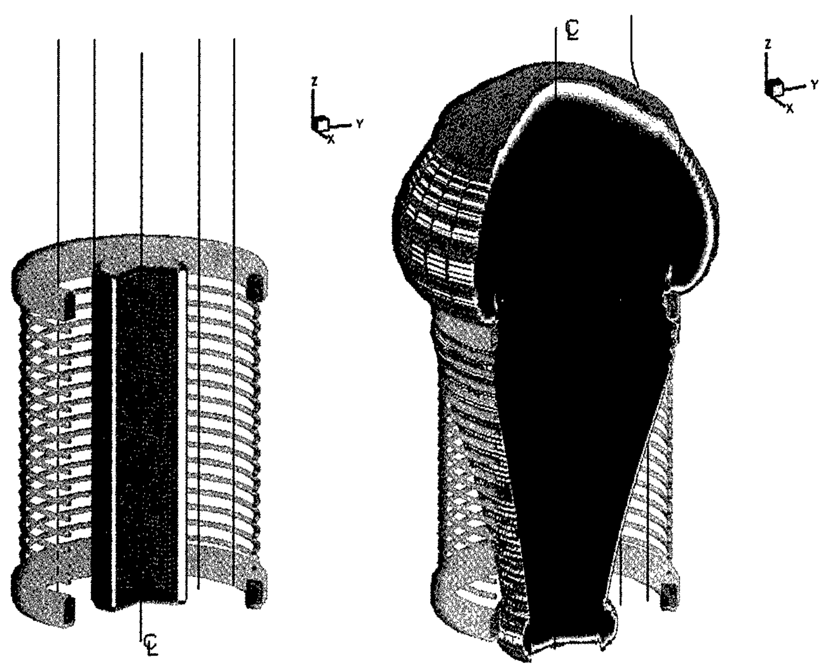
Research Objective: To simulate complex, three-dimensional (3-D) hydrodynamic and dense plasma phenomena with sufficient resolution to perform virtual prototyping of a class of explosive pulsed-power devices to power a variety of advanced weapons. In these devices, an explosive material is detonated so as to compress a volume filled with a magnetic field. This compression amplifies the field, creating an electrical voltage that can be used to power some plasma-based weapons. Three-dimensional simulations of real devices require greater memory and operations per second than are currently available on a single computer node. Our 3-D magnetohydrodynamics code MACH3 is designed to run on many of the scalable computing resources available to DoD and allows us to perform physics simulations that were never before possible.

Methodology: MACH3 uses a domain decomposition scheme of arbitrarily shaped hexahedral blocks on a 3-D mesh. The blocks are split among available compute nodes by the user so that each node may "own" one or more computational blocks. Thus for a problem with *N* blocks, MACH3 can run using any combination of one to *N* nodes. The message-passing interface (MPI) is used for sharing neighbor data between blocks that are on different compute nodes. Because MPI is an industry standard, its use ensures portability of the code to most HPC platforms.

Results: We ran a 60-block simulation of the hydrodynamics of an explosive flux compression generator with an outer helical coil on 28 nodes of the P2SC SP at MHPCC that was nearly one million cells and took almost 2 Gbytes of memory. The largest amount of memory on any one node is 1 Gbyte, so this problem would not run in serial. We estimate that if we could run this problem in serial, it would take a month to complete. Using 28 nodes, the problem ran to completion in only two days. The figure shows the explosive armature before detonation and 40 microseconds into the detonation, by which time the top portion of the armature has hit the helical field coil.

Significance: The ability to compute large, complex, 3-D problems on distributed computing platforms is enabling us to perform entire magnetohydrodynamic simulations of explosive generators. Portable, high energy density, compact pulsed-power devices like explosive magnetic generators will play key roles in the development of some of the next-generation weapons concepts.

JWCO: Precision Force



Snapshots of the initial (left) and intermediate (right) state from a MACH3 simulation of an explosive helical magnetic generator. The image was created with Tecplot from binary data produced during execution of MACH3.

FISC Solves Electromagnetic Problems of Unprecedented Size

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S.W. Lee
DEMACO Inc., Champaign, IL

HPC Computer Resource: SGI Origin 2000 [ASC MSRC]

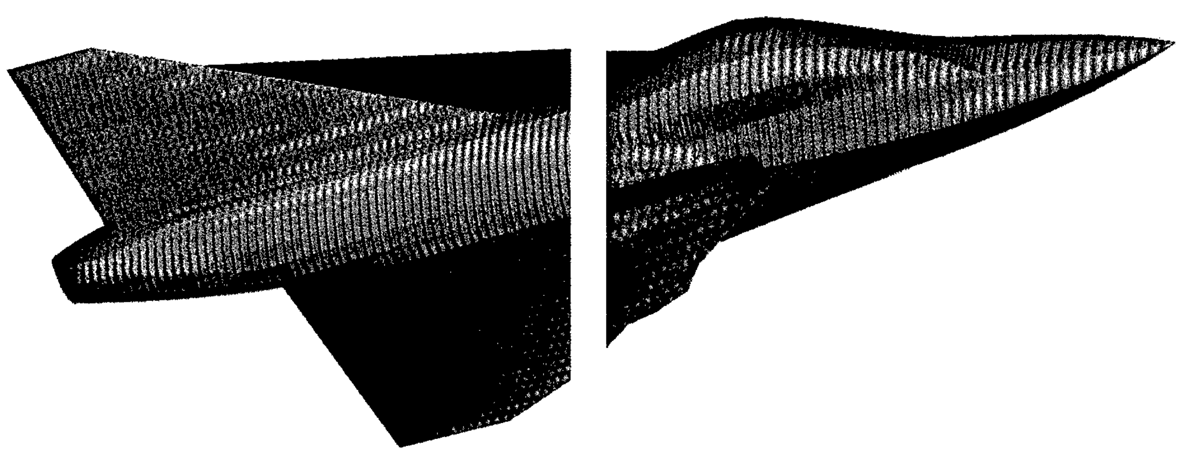
Research Objective: To develop a new knowledge base that will allow computer solutions to electromagnetic problems of unprecedented sizes and complexity. The resultant codes and algorithms with reduced computational complexity and memory requirements will significantly alter the manner in which computers are used in the design of antennas, radar cross-section (RCS) reduction of aircraft, high-speed circuits, remote sensing, and related applications.

Methodology: FISC is designed to compute the RCS of a three-dimensional complex target. The problem is formulated by the method of moments. The resulting matrix equation is solved iteratively by the conjugate gradient (CG) method. MLFMA is used to speed up the matrix-vector multiply in CG. Both complexities for the CPU time per iteration and memory requirements are order of $N \log N$, where N is the number of unknowns and is proportional to the surface area of the target.

Results: The electromagnetic problem for aircraft like VFY218 at 1 GHz can be solved on a supercomputer with the conventional method. FISC can solve it on workstations. Using the SGI Origin 2000, we are the first group to successfully solve the problem for aircraft like VFY218 at 2 and 3 GHz, where more than two million unknowns are involved. Savings of the computation time and memory over the conventional method is more than several orders of magnitude.

Significance: The problems solved by FISC are the largest ever solved by numerically accurate methods. FISC bridges the gap between the conventional accurate methods for low frequency and the approximate methods for high frequency. It can be used to validate codes for high frequency and to calculate RCS and synthetic aperture radar images of complex targets. In addition to calculating RCS, computational electromagnetics impacts the design of computer chips, antennas and telecommunication systems, bioelectromagnetics, remote sensing, oil and mineral exploration, and microelectromechanical sensors.

JWCO: Combat Identification, Electronic Combat



Electric current distribution on parts of VFY218 at 2 GHz

Highly Accurate Schemes for Radar Signature Determination

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HPC Computer Resource: Cray C90 [ASC, CEWES, and NAVO MSRCs] and Cray Y-MP [CEWES MSRC]

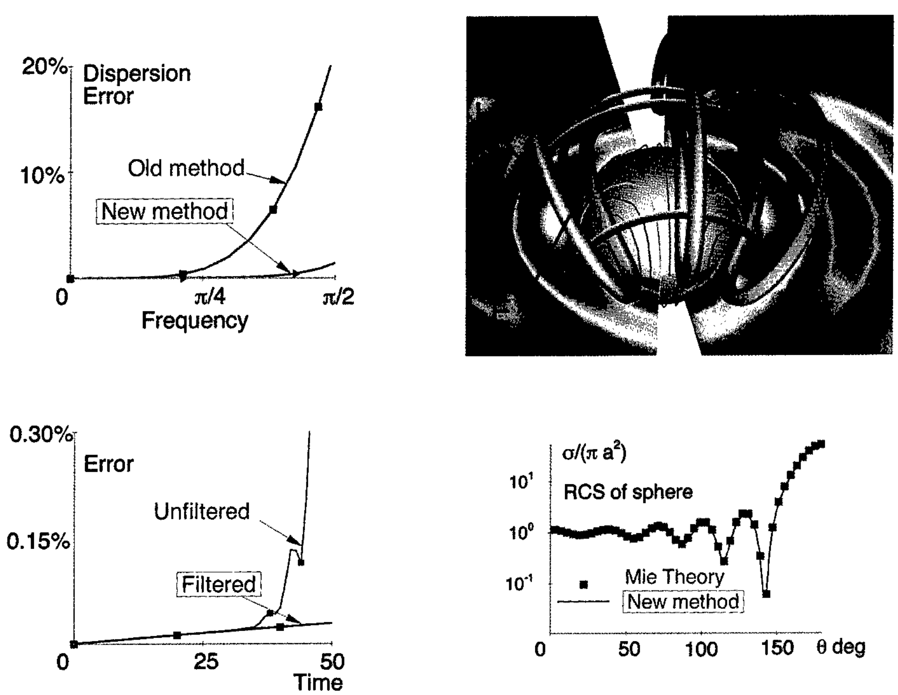
Research Objective: Numerical determination of the radar cross section (RCS) of military aircraft is of immense importance in the design and analysis of low-observable vehicles. Present computational technology cannot routinely provide such results because of the intensive nature of this endeavor. The goal of this effort is to alleviate this difficulty by developing more accurate, and consequently more efficient, methods. These results have direct impact on the DoD Challenge Project to analyze the RCS of the B-1B.

Methodology: The electromagnetic phenomena under consideration are governed by Maxwell's equations, which are solved with the time-domain finite-volume formulation. The solution reconstruction procedure adopts the primitive function approach followed by the application of fourth- and sixth-order accurate centered "compact"-difference-based (or Pade-type) methods. The classical fourth-order Runge-Kutta method is used for time integration.

Results: This effort developed, implemented, and tested the new scheme in a computer code capable of handling general curvilinear meshes. Particular emphasis was placed on avoiding excessive stretching error, which can rapidly degrade accuracy. The graphic shows the superiority of the new method. To suppress late-time numerical instabilities, a sophisticated spatial filter scheme of up to tenth-order accuracy and relatively small computational overhead was developed. The composite algorithm was then tested in a variety of representative but computationally intensive problems requiring Cartesian as well as curvilinear meshes, including some with mesh singularities.

Significance: The highly accurate method developed in this work is estimated to improve computer processing efficiency while simultaneously reducing the required memory by factors of at least sixteen and eight respectively. The implementation of this scheme in the B-1B signature computation will greatly reduce the resources required and will further expand the scope of that study. An additional payoff accrues from the fact that the schemes have been transitioned to the analysis of fluid dynamic phenomena where they show substantial promise.

JWCO: Information Superiority, Combat Identification



High-order algorithm (top left) with advanced numerical filtering (bottom left) constitutes a superior scheme for electromagnetic fields (top right) and RCS computations (bottom right).

Broadband Electromagnetic Simulation on Unstructured Grids

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H. Wang
Naval Air Warfare Center, China Lake, CA

HPC Computer Resource: IBM SP [MHPCC DC and ASC MSRC] and Intel Paragon [ASC MSRC]

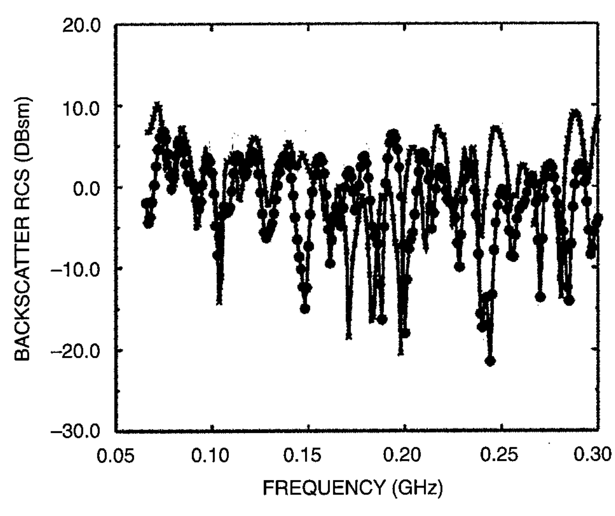
Research Objective: To develop a scalable solver for the time-dependent Maxwell equations on unstructured grids to provide quick turnaround in computing broadband radar scatter; radar range design and simulation; and the effects of high-power microwaves, electromagnetic interference, and electromagnetic pulse. Performance should scale as the number of processors on all parallel architectures, from massively parallel computers to workstation clusters. The objective of this two-person level of effort is to extend results obtained over a 10-year period in time-domain electromagnetics.

Methodology: The solver integrates Maxwell's equations forward in time for each finite-volume cell in an unstructured grid. For complex targets, such as fighter aircraft, grids are automatically generated and fitted to the target surface from a standard CAD database. Recursive spectral bisection provides good load balance with communication overhead of a few percent. Accurate propagation of waves over the target through the variable geometry of unstructured cells is the major challenge for the method. Work is also ongoing to improve and extend the grid generator UNISG and the run environment UNSPREP.

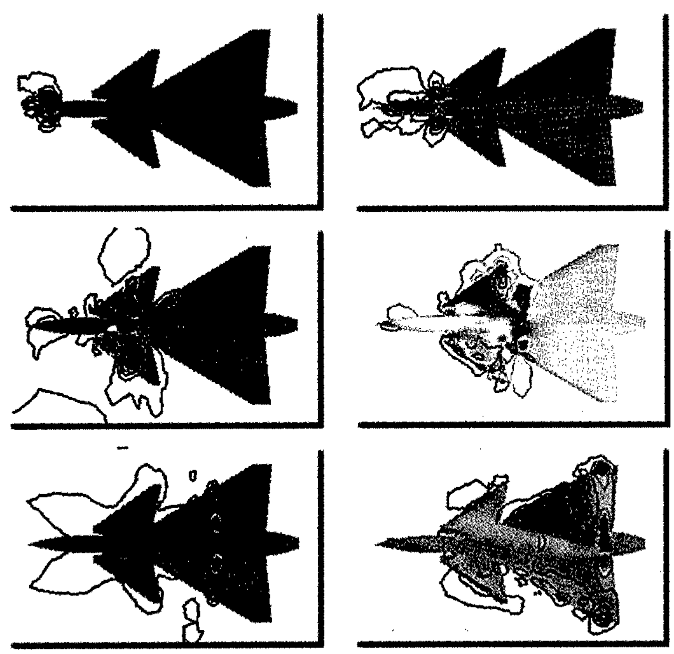
Results: The solver UPRCS is based on the codes RCSMPP and RCSUN, which have shown excellent scalability on a wide range of platforms. The present stage of implementation of UPRCS is giving good results for the radar cross section (RCS) of difficult target benchmarks. The first pulse calculation of backscatter RCS for a fighter aircraft using UPRCS is shown below for nose-on incidence. The figures illustrate the passage of a vertically polarized plane pulse over the VFY218, showing the total horizontal electric field at each instant. The inset graph shows a comparison of the measured and calculated RCS from 50 to 300 MHz, derived from a single time integration. The grid was designed to be accurate at 100 MHz, which is why the results begin to disagree above 200 MHz.

Significance: Computational electromagnetics (CEM) is a critical technology in the development of Precision Force elements through supercomputing. As we transition from the present Gflops to next-generation Tflops computing, CEM will become integral to aerospace design not only as a stand-alone technology, but also as a part of the multidisciplinary coupling that leads to well-optimized designs.

JWCO: Precision Force, Electronic Combat



Comparison of measured (line) and calculated (graph) (dots + line) RCS



VFY218 pulse calculation 100 MHz grid, VV-pole, nose-on incidence

Overset Grids for Computational Electromagnetics

Capt. D.C. Blake and Maj. T.A. Buter, U.S. Air Force
Air Force Institute of Technology, Dayton, OH

HPC Computer Resource: Intel Paragon and IBM SP [ASC MSRC] and Cray T3D [AFDTC DC]

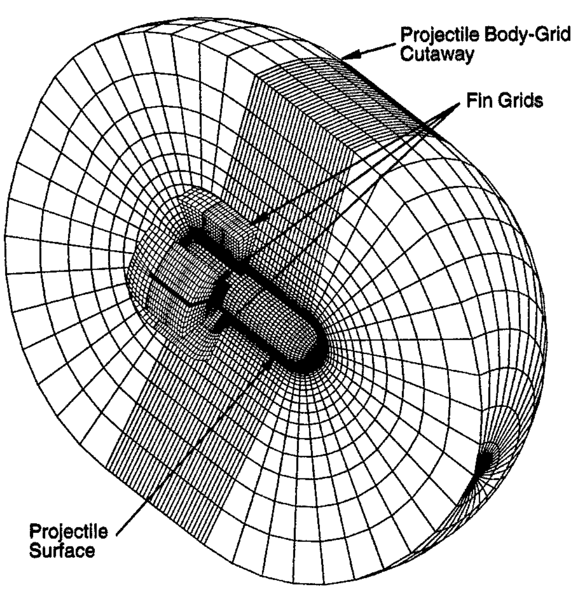
Research Objective: To investigate the feasibility of using overset grids in conjunction with a finite-volume time-domain (FVTD) Maxwell equations solver for conducting electromagnetic scattering and wave propagation simulations on massively parallel computing platforms.

Methodology: The three-dimensional Maxwell equations are solved explicitly over a computational domain that is formed by dividing a complex geometry into a series of components and then generating a body-conformal structured grid around each component. The resulting grids are allowed to arbitrarily overlap and are thereby combined to form a globally unstructured grid. A parallel implementation is achieved by partitioning the computational domain after forming the single global grid, which results in both improved load balance and a marked reduction in intergrid associated communication requirements.

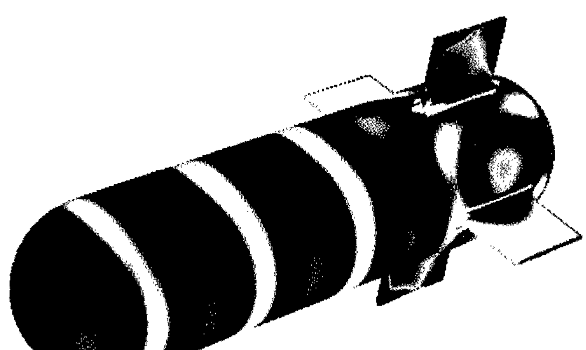
Results: Results from a large number of scattering and wave propagation simulations conducted using overset grids show that the overset grid algorithm can produce solutions of comparable accuracy to those obtained using nonoverlapped grids, while greatly simplifying the often complex grid-generation procedure. Furthermore, this algorithm has proven to be highly scalable over a wide range of problem sizes, routinely achieving parallel efficiencies in excess of 90% on up to 128 processors.

Significance: As computational capabilities evolve, numerical simulation of electromagnetic phenomena involving geometrically complex weapons systems becomes an increasingly viable design tool; however, modeling such complex geometries can be extremely labor intensive. The ability to use flexible gridding approaches such as overset grids in conjunction with massively parallel computers dramatically extends the viability of the FVTD methodology.

JWCO: Electronic Combat



Overset grid configuration



Contours of scattered electric field

Finned projectile scattering simulation

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Climate/Weather/ Ocean Modeling

Climate/Weather/Ocean Modeling and Simulation (CWO) is concerned with the accurate numerical simulation and forecast of oceanic and atmospheric variability for both scientific and operational use. CWO is used on a daily basis within DoD for safety in flight, safety at sea, search and rescue, mission planning and rehearsal, optimal aircraft and ship routing, antisubmarine warfare, expeditionary warfare, and weapon system design.

Several of the stories directly address the impact of model resolution on model accuracy or forecast skill. The world's ocean circulation has been modeled at a 1/16-degree resolution, the highest resolution global ocean model yet attempted. In a related effort, it was discovered that a resolution of 1/32 degree was required to reliably simulate the path of the Gulf Stream between Cape Hatteras and the Grand Banks. HPC resources have been used to investigate the importance of resolution and ensemble forecasts on predicted storm path and intensity. The accurate forecast of tropical cyclone track and intensity is clearly of great importance to both DoD and this nation. The influence of islands on oceanic circulation has been studied by using a multiyear simulation of the circulation in the Pacific Ocean at a 1/8-degree resolution. Two of the success stories deal with efforts to create numerical models on tactical scales. An assimilation technique has been developed to initialize water vapor distributions in theater-scale meteorological forecasts. Tactical-scale cloud forecast systems such as this can have a dramatic effect on aircraft safety, materials selection, and communications. A multiblock coastline-fitted nearly orthogonal curvilinear gridding package has been developed to support tactical-scale application to operations littoral-mine warfare, special operations, and expeditionary warfare. A parallel ocean-ice model has been developed that has applications to arctic undersea warfare and submarine search and rescue. These success stories illustrate both the wide range of applications-basic research to operational forecast system development and the grand challenge nature of the CWO efforts.

Joseph W. McCaffrey, Jr.
Naval Research Laboratory
Stennis Space Center, MS
CTA Leader for CWO

First 1/16-Degree Global Ocean Model

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Naval Research Laboratory, Stennis Space Center, MS

HPC Computer Resource: Cray T3E [CEWES and NAVO MSRCs]

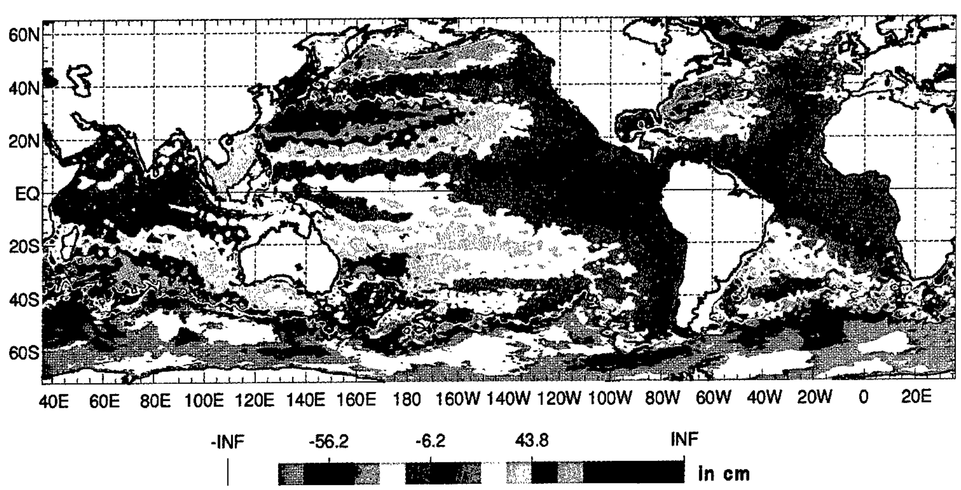
Research Objective: To coordinate efforts on the DoD HPC Challenge problem of eddy-resolving global and basin-scale ocean modeling and prediction. This includes increased understanding of ocean dynamics, model validation, naval and global change applications, oceanic predictability studies, and observing system simulation studies.

Methodology: The NRL Layered Ocean Model is typically tens to hundreds of times more efficient than other global ocean models. This is primarily because Lagrangian layers are used in the vertical direction and a semi-implicit time scheme makes the time step independent of all gravity waves (but requires the solution of Helmholtz equations). The Helmholtz solver is very efficient but has large memory requirements. The 1/16-degree global ocean model requires about 5 GigaWords of memory. The Cray T3Es have 64 MegaWords of memory per processor, so the global model must use at least 80 processors. Many more processors can be used without significant loss of efficiency, e.g., 224 T3E processors run 1.95 times faster than do 122 processors.

Results: The NRL global ocean model was integrated from rest to statistical equilibrium, driven by monthly climatological winds at progressively higher resolutions (1/2, 1/4, and 1/8 degree) for 847 model years. The first extension at 1/16 degree was performed under a DoD HPC Challenge Project, including 68 model years at 1/16-degree resolution and two simulations run from 1979 through 1996 forced by 6 hourly reanalysis winds from the European Centre for Medium-Range Weather Forecasts. The resolution increase allows sharper definition of oceanic fronts and better simulation of meandering currents and the mesoscale eddy field (see figure). The identical twin interannual simulations help distinguish between deterministic and nondeterministic model responses to the atmospheric forcing and are valuable in model-data comparisons and dynamical studies of oceanic anomalies.

Significance: These 1/16-degree simulations have the finest resolution ever achieved on global ocean models. The best resolution previously obtained with global ocean models (outside of NRL) was the approximately 1/5-degree resolution achieved by a research group at Los Alamos National Laboratory. By a careful choice of algorithms, we have been able to run simulations on existing supercomputers. These supercomputers operate at much less than 1 Tflop/s sustained speed for ocean models. Eddy-resolving models are an important milestone on the road to global ocean modeling and prediction systems. Applications include military operations, such as sealift ship routing, search and rescue, antisubmarine warfare, coastal and mine warfare, and commercial applications, such as ship-routing, fisheries forecasts, and global ocean simulation and prediction, e.g. pollutant spill risks, El Ninõ forecasting, ocean observing system simulations, and global change studies.

JWCO: Precision Force



Sea surface height snapshot for 26 March 1990 simulated by the NRL global ocean model with 1/16-degree horizontal resolution for each variable. Contour interval is 12.5 cm.

Realistic Simulation of the Gulf Stream Pathway Using a 1/32-Degree Atlantic Model

H.E. Hurlburt and P.J. Hogan
Naval Research Laboratory, Stennis Space Center, MS

HPC Computer Resource: Cray T3D [AFDTC DC], Cray T3D [ARSC], Cray T3E and IBM SP [CEWES MSRC], and Cray T3E and T90 [NAVO MSRC]

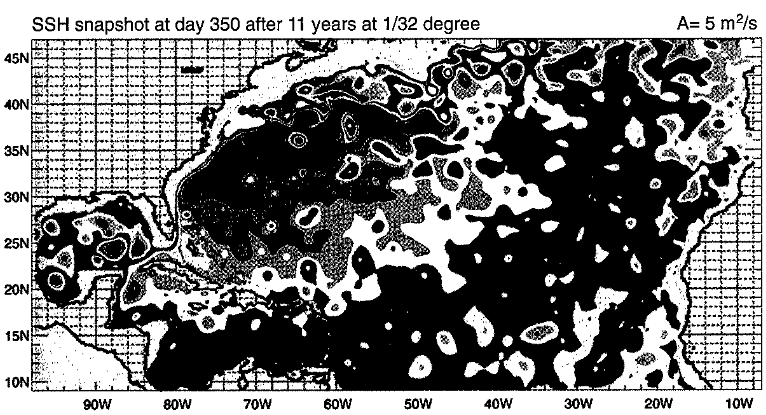
Research Objective: To develop an eddy-resolving global and basin-scale ocean nowcast/forecast system. This includes an understanding of ocean dynamics, model validation, naval and global change applications, oceanic predictability, and observing system simulation.

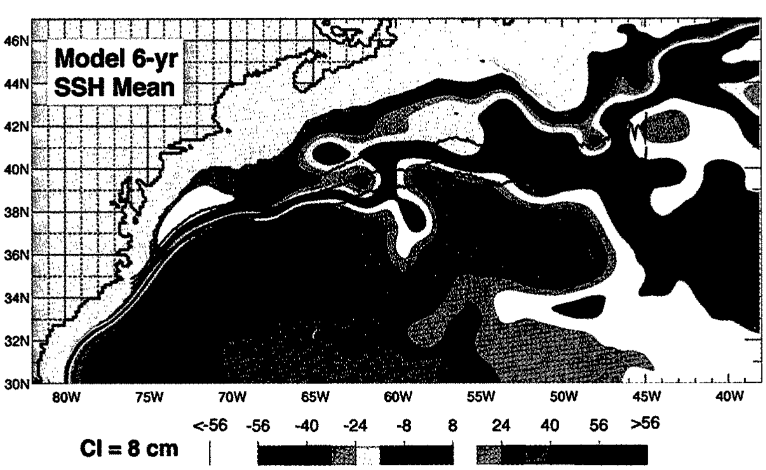
Methodology: We have developed a scalable portable version of the NRL Layered Ocean Model that can run efficiently and interchangeably on any HPC system configured for large applications. For scalability to multiple processors, the model uses the technique best suited to each machine type: autotasking on the Cray T90, MPI message passing on the IBM SP, and SHMEM one-sided message passing on the Cray T3D/T3E.

Results: The NRL model has been used to simulate the Atlantic Ocean (9° N to 51° N) from 1/2 (56 km) to 1/32-degree (3.5 km) resolution with five layers in the vertical. Resolution of 1/32 degree is the highest ever achieved for modeling a major ocean basin. Major changes from linear solutions are required for realistic nonlinear simulation of the Gulf Stream pathway between Cape Hatteras and the Grand Banks. This was robustly achieved only at 1/32-degree resolution (see figure). This resolution also increased the realism of the large-scale gyre, the eddy field, and the flow transported through passages in the Caribbean Sea and the Gulf of Mexico.

Significance: Realistic simulation of Gulf Stream separation from the coast at Cape Hatteras and its pathway from Cape Hatteras to the Grand Banks is a "Holy Grail" problem in ocean modeling, where many have tried and failed. The NRL 1/32-degree subtropical Atlantic model is the first to achieve this in a robust fashion. We found that upper-ocean topographic coupling via mesoscale flow instabilities is crucial for accurately simulating the Gulf Stream. Eddy-resolving ocean models are an important milestone on the road to global ocean monitoring and prediction systems. Applications include assimilation and synthesis of global satellite surface data; optimum track ship routing; search and rescue; antisubmarine warfare and surveillance; tactical planning; high-resolution boundary conditions for even higher resolution coastal models; inputs to ice, atmospheric, and biophysical models and shipboard environmental products; simulated environments; pollution and tracer tracking; and inputs to water quality assessment.

JWCO: Precision Force, Joint Readiness and Logistics





Mean sea surface height in the Gulf Stream region from the 1/32-degree Atlantic model compared with the Gulf Stream northern edge from satellite infrared imagery (1982 to 1996 mean)

High-Resolution Ensemble Forecast of a Land-Falling Storm

T.N. Krishnamurti
Florida State University, Department of Meteorology, Tallahassee, FL

HPC Computer Resource: Cray C90 [CEWES MSRC]

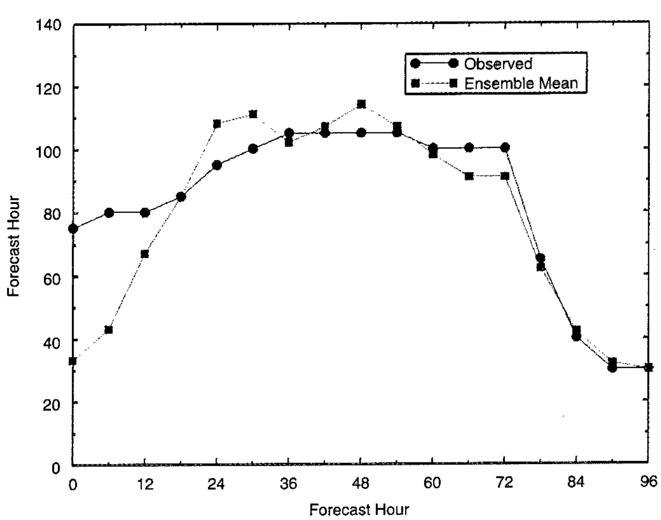
Research Objective: To use high-performance computing to produce realistic intensity forecasts of hurricanes. Hurricane Fran made landfall over North Carolina on September 6, 1996. This storm's intensity was category 3 (maximum winds of around 110 knots). A hierarchy of Florida State University's (FSU) weather forecast models were used toward a successful forecast of the intensity of this storm. This forecast system consists of (a) a global model at resolution T106 (roughly 100 km horizontal resolution) that provides the base state and boundary condition for the high-resolution model; (b) a global model that includes rain-rate initialization (physical initialization), run at resolution T170 (horizontal resolution 70 km) that provides the initial perturbation for the high-resolution regional spectral model; (c) a six-day forecast using a one-way nested high-resolution regional spectral model (horizontal resolution 0.5° latitude/0.5° longitude); and (d) ensemble forecasts of hurricane tracks made using an empirical orthogonal function (EOF)-based perturbation (of storm location, intensity, temperature, and wind speed), averaged to provide our system's best forecast track and intensity.

Methodology: The numerical models applied in this study use the spectral modeling approach along with Fourier-Lengendre and double Fourier basis functions for the global and regional models, respectively. These models include a complete array of physics algorithms for the planetary boundary layer, convection, radiative transfer, clouds, and land-air-sea interactions.

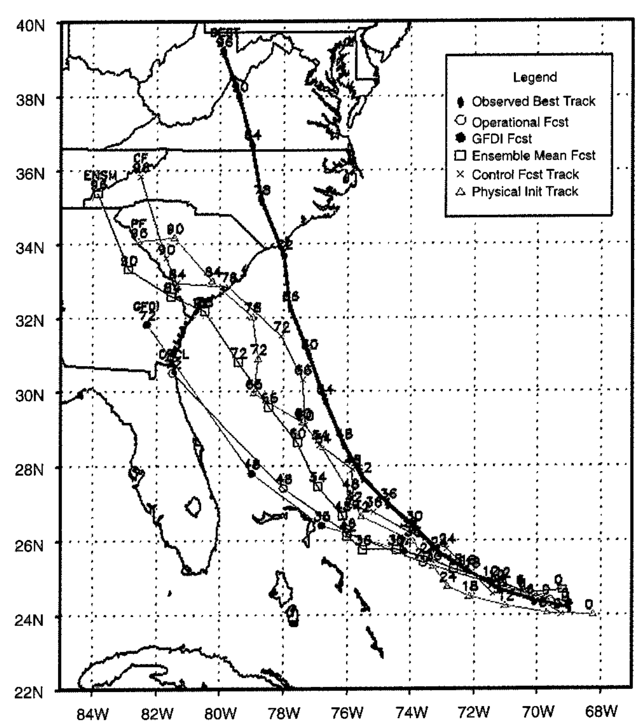
Results: The figures show the track and intensity forecasts from our system for Hurricane Fran starting on September 3, 1996. The track forecast through day 4 was best provided by the various FSU models that showed somewhat better skill compared to other models and the official forecast. The category 3 storm's intensity and the weakening of the storm during the last 36 hours were predicted extremely well. The success of this forecast is largely attributed to physical initialization and the high-resolution computations using the regional model.

Significance: The promising results obtained for Hurricane Fran and an earlier storm (Hurricane Opal, of 1995) call for a major concerted research effort on a larger sample of storms. These results foretell major improvements in forecasting land-falling storms.

JWCO: Joint Readiness and Logistics



Storm intensity vs forecast time



Ensemble of predicted tracks

Hurricane Fran tracks and intensity for prediction beginning September 3, 1996 0000Z

The Influence of Islands on Local Circulation of the Pacific Ocean

J.J. O'Brien
Florida State University, Tallahassee, FL

HPC Computer Resource: Cray C90 [NAVO MSRC]

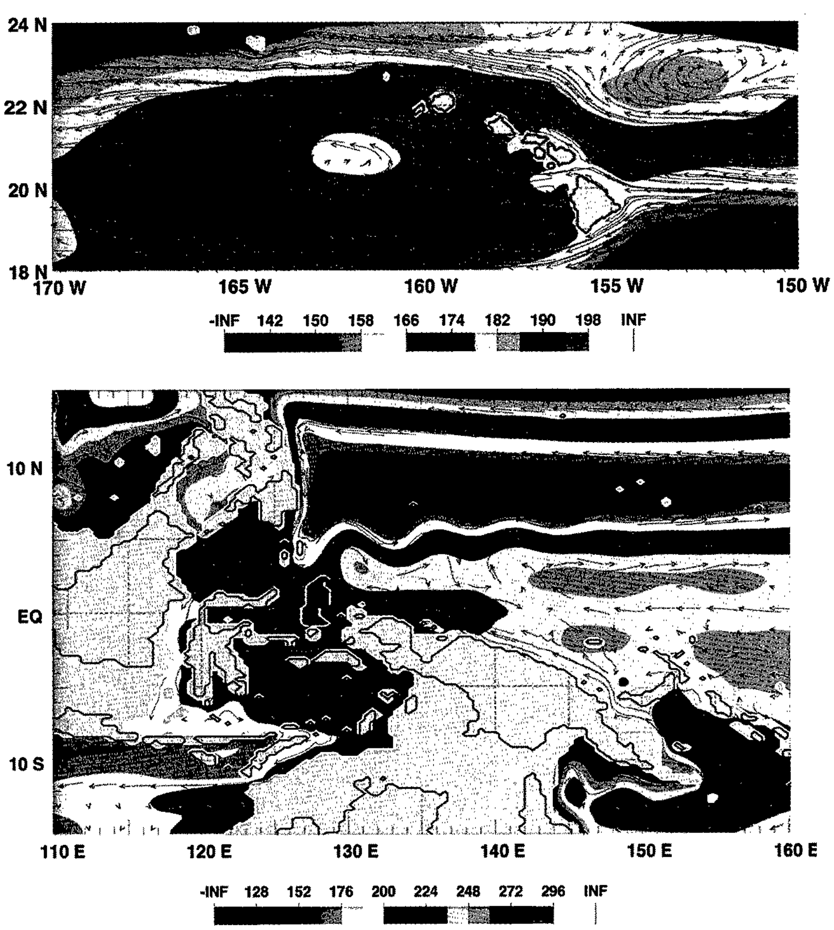
Research Objective: To investigate the dynamic effect of large island masses on the currents of the upper Pacific Ocean.

Methodology: The Naval Research Laboratory high-resolution, multilayer Pacific ocean model is driven by a modified version of the European Centre for Medium-range Weather Forecasts surface winds corresponding to 1981 through 1994. In this cooperative effort, an NRL ocean modeling team does the computations and FSU scientists analyze the output.

Results: This collaborative study focused on two island regions, the Hawaiian Islands and Indonesia, especially Halmahera of the Philippine Islands. The westward ocean current impinging on Hawaii is found to be diverted northward and southward around Hawaii. The dramatic result is a shadow zone in the lee of Hawaii that contains energetic ocean eddies comparable in size to the island of Hawaii. Halmahera Island is found to prevent flow of South Pacific water into the Celebes Sea, diverting some of it southward through the Seram and Banda Seas. Halmahera impacts the lower thermocline and intermediate water pathways throughout the year, but affects the surface layer only during the northern hemisphere's spring and fall.

Significance: This project was conducted as a cooperative effort between Naval and academic personnel. Topography has been shown to have a powerful effect on ocean circulation in the regions of study. Naval operations can use this information to better understand the local environment, thereby enhancing countermine measures and deployment.

JWCO: Joint Countermine



In the ocean model results from the regions of Hawaii (top) and Indonesia (bottom), surface currents are represented by arrows and layer thickness is represented by color. In the bottom figure, Halmahera Island is highlighted in red near the center of the domain.

Specification of the Spatial Distribution of Water Vapor Using Visible-Band Geostationary Satellite Data

G.D. Modica and A.E. Lipton
Air Force Research Laboratory, Hanscom AFB, MA

HPC Computer Resource: Cray C90 [CEWES and ASC MSRCs]

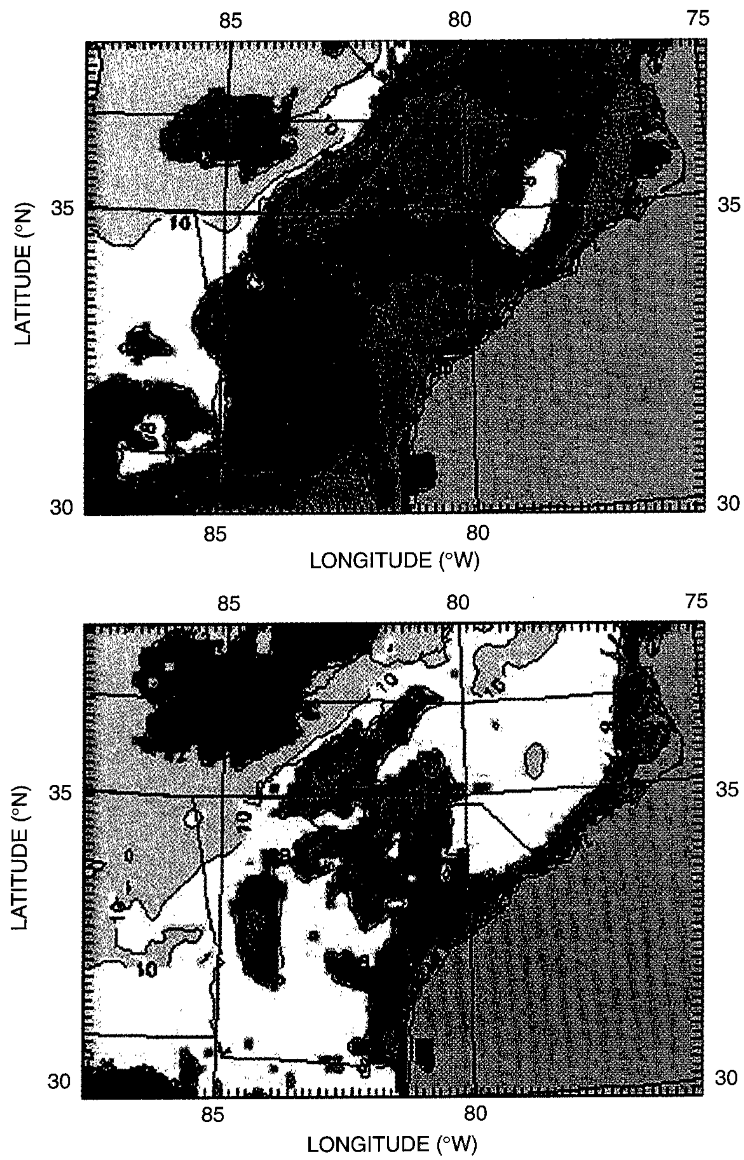
Research Objective: To produce optimal analyses of water vapor and improve subsequent forecasts of convective clouds within theater-size domains.

Methodology: Within a numerical weather prediction model-based analysis, the model's capability to simulate horizontal variations in the surface heating field was improved by specifying the positions of clouds based on satellite observations. In addition, the model's radiation parameterization was optimized to minimize the departure of the resulting surface insolation from ground truth.

Results: Results indicate that the procedure enables the model to produce more accurate shelter height temperatures, moisture convergence patterns, and surface winds than it can without satellite data input (see figure). These positive effects appear to be maintained throughout integration of a 9-hour forecast.

Significance: Convection can be a dominant physical process in theater-size domains and is also a necessary ingredient in the production of cumulus clouds in the troposphere. At the same time, its chaotic behavior makes it one of the most difficult physical processes to predict. This study deals with improving the capability of atmospheric models to predict convection. If cloud forecasts from numerical weather prediction models can be improved significantly, the effect will be one of force multiplication, as combat resources are not wasted on failed missions owing to poor line-of-sight visibility. Better predictions of clouds, precipitation, and associated aviation impact variables (e.g., icing and downbursts) are also relevant to the civilian aviation community and other general interests affected by the weather. Furthermore, the capabilities developed through this research will assist the modeling and simulation community by enabling the introduction of more realistic weather inputs into simulation models.

JWCO: Precision Force, Joint Readiness and Logistics



Change in temperature (°C) 2 m above ground from 0700 to 1300 EST; contours every 2°C. Upper figure is based on data from a control analysis that used no satellite data; lower figure is based on an analysis that assimilated visible and infrared imagery from a geostationary satellite (GOES-7). The technique used in the lower figure more accurately accounts for the effects of observed clouds on the evolving meteorological patterns. A more accurate depiction of these patterns could result in better predictions of atmospheric parameters that impact Air Force operations.

A New Advance in Coastal Ocean Modeling: Application of the Grid Generation Technique

L. Ly
Naval Postgraduate School, Monterey, CA
P. Luong
Stennis Space Center, MS

HPC Computer Resource: Cray C90 [NAVO MSRC]

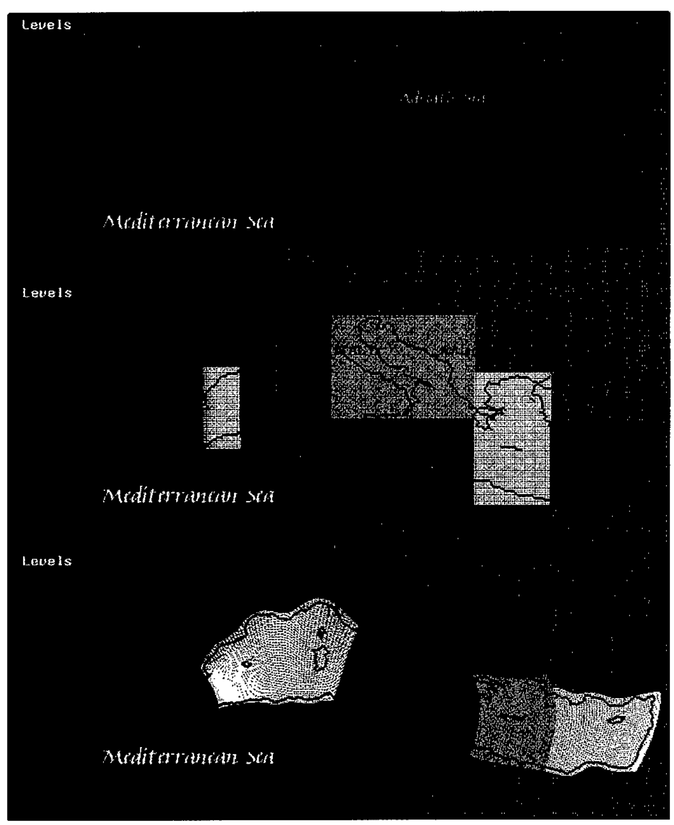
Research Objective: To develop a technique for numerically generating multiblock coastline-fitted, nearly orthogonal curvilinear (MUBCOSFNOC) grids. These will improve the accuracy of coastal ocean model forecasts and simulations of the evolution and interaction of multiscale physical phenomena of coastal ocean structures related to complex coastlines, open boundaries, and bottom topography, and will save computing resources.

Methodology: Numerical grid generation is used to produce MUBCOSFNOC grids, which are coupled to a state-of-the-art coastal ocean model. We developed a grid package that allows the model to be coupled with the model grids. Our coastal ocean model code is written for multiblock grids.

Results: Our study shows that the traditional single-block rectangular grids are not well suited to modeling coastal regions, which have complicated coastlines, bottom topography, and multiscale physical phenomena. These grids can lead to poor accuracy of the numerical solution and nonoptimal compromise between accuracy and computer resources. An effective coastal model represents the thermodynamics of the coastal ocean flow on the model grids, including the effects of complicated features such as coastlines, bottom topography (submarine canyons, seamounts, narrow straits), and multiscale physical phenomena. These problems require a model grid system that is more efficient than a traditional single-block rectangular grid, model grids that provide better resolution of coastlines, boundary conditions, and multiscale physical phenomena, and save computer resources. Our MUBCOSFNOC grids enhance model numerical solutions by better treating coastlines, open boundaries, bottom topography, and multiscales of physical phenomena. These grids are smooth, they present no problems in multiblock (subregion) interactions such as nesting, and they are effective and easy to use in parallel computing.

Significance: Improvements in the accuracy of coastal ocean circulation simulations and forecasts are necessary for the Navy, Marine Corps, and Army in littoral or coastal operations and coastal warfare such as naval mine, diving, or special warfare. These improvements have enabled use of higher resolution models and multiscale, more realistic ocean simulation.

JWCO: Precision Force, Joint Countermine



The Mediterranean Sea coastlines modeled using a single-block traditional rectangular grid (top), a nine-block orthogonal grid (middle), and an eight-block, curvilinear, nearly orthogonal grid (bottom).

Advanced Modeling of the Arctic Ocean and Sea Ice in Support of Global Climate Studies

W. Maslowski and A.J. Semtner
Naval Postgraduate School, Monterey, CA

HPC Computer Resource: Cray T3D and T3E [ARSC]

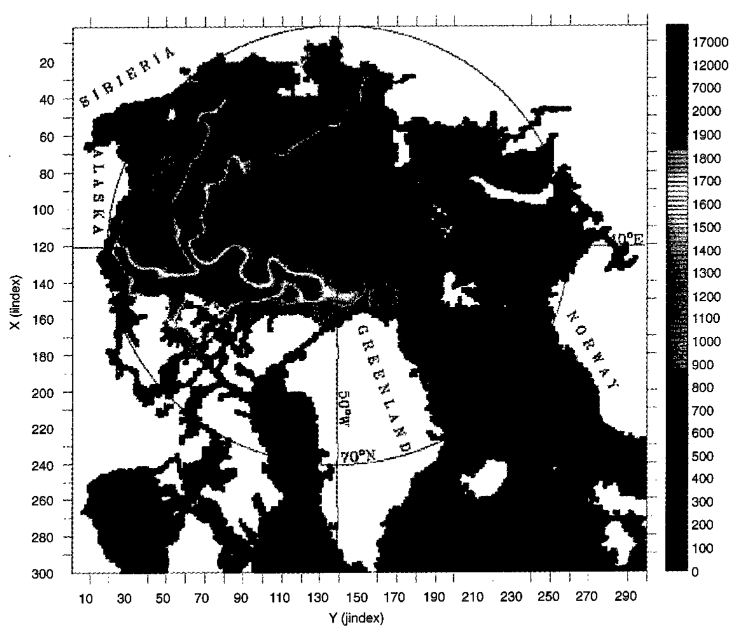
Research Objective: To apply HPC to more realistically model the Arctic Ocean's physics and integrate the resultant data into global climate models. The polar regions gained much attention after many climate models indicated that the largest response to climate change will occur there. The same studies have been criticized for basing some of their biggest predicted climate changes on a poorly observed region (i.e., the Arctic) and for having those predictions depend critically on processes that are not yet well modeled, including clouds, snow, and surface energy budget feedbacks as well as heat, salt, and fresh water balance. The Arctic Ocean is the ocean from which most new insights relevant to climate change are likely to be obtained when its circulation and connections to other oceans are successfully modeled. Different predictions could result from climate models should the polar regions be more realistically simulated.

Methodology: The original Parallel Ocean Program (POP) was developed for the global ocean (with the Arctic Ocean excluded) at the Los Alamos National Laboratory on the CM-200. We converted and optimized the code to run on the Cray T3D in a joint effort with Los Alamos, the National Center for Atmospheric Research, and Cray and then adapted it for the Arctic Ocean with a horizontal resolution of 1/6 degree and 30 vertical levels to more realistically represent mixing and water mass formation in the Arctic Ocean.

Results: A 200-year integration resolving key features of the flows and current interactions within the Arctic Ocean was completed. Arctic ocean currents are topologically controlled and are typically 100 km wide or less. Eddies simulated in the current model are on the order of 100 km. Ice thickness and concentration depend on the oceanic and atmospheric fields and on the behavior of eddies. Predictions of ice thickness and concentration have matched well with actual events. Several simulations of both active and passive tracers investigated Pacific water entry and circulation, nuclear contaminant dispersion, the fate of river runoff, and overall Arctic Ocean fresh water circulation.

Significance: The model provides a testbed for including advanced submodels of sea ice, a mixed layer, tidal mixing, and deep convection in the model to realistically represent physics. It has been coupled to the global 1/4-degree Semtner-Chervin model to allow interactions between the Arctic and the world's ocean, thereby allowing full-physics global integration in future climate studies. A fully global ice-ocean model including the Arctic Ocean with averaged horizontal resolution of 1/3-degree is being developed to run on the Cray T3E at ARSC.

JWCO: Precision Force, Joint Readiness and Logistics



Distribution of fresh water into the Lena River after 12 years of integration in the Active River Tracer Experiment

Simulating the Response of Drifters to Deep Convection

R.W. Garwood, Jr., L. Jiang, and R. Harcourt
Naval Postgraduate School, Monterey, CA

HPC Computer Resource: Cray C90 and T90 [NAVO MSRC]

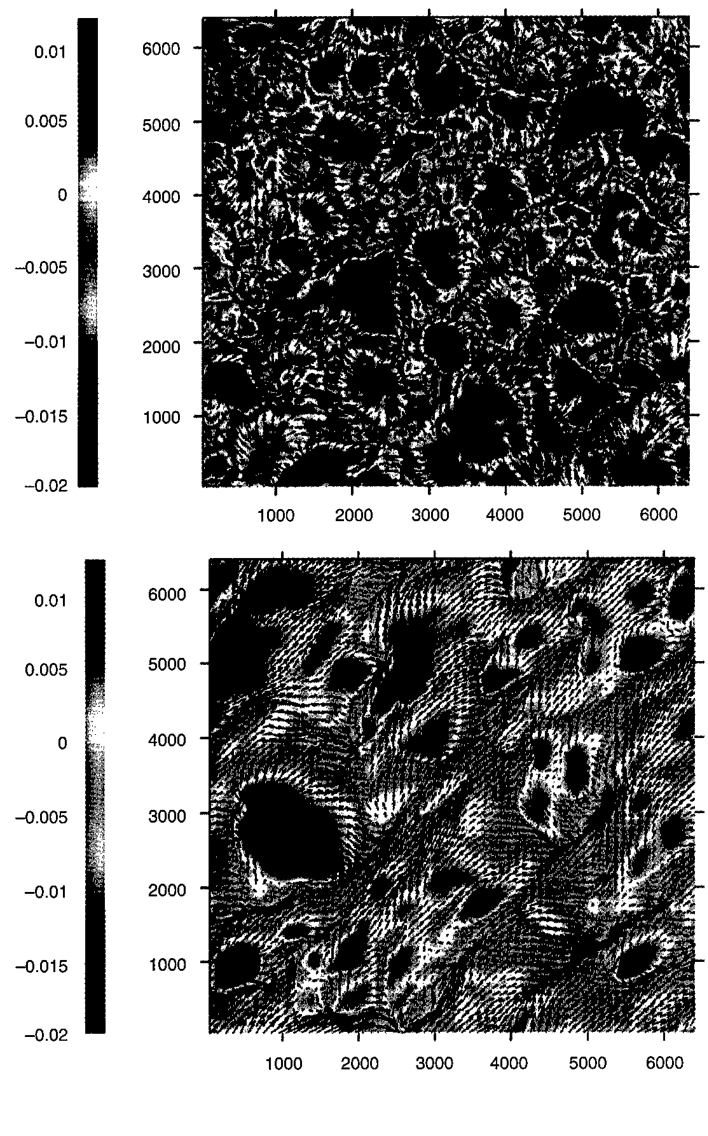
Research Objective: To simulate the response of Lagrangian drifters to deep oceanic convection in the Labrador Sea. These simulations are being used to interpret the data recorded by drifting sensors and to test the strategies and combinations of drifter types deployed for the Office of Naval Research Accelerated Research Initiative in Labrador Sea deep convection.

Methodology: Large-eddy simulation (LES) of Labrador Sea convection is performed with an embedded Lagrangian drifter model (LDM). The LES model uses a modeled subgrid energy to compute a local nonlinear viscosity for turbulence closure. The LDM interpolates the discretized field and computes float trajectories as the LES fields evolve. The code uses parallel and vector library routines, auto-parallel compilation, and asynchronous buffering to maximize the efficiency with which it uses CPU cycles and to minimize the demands on core memory space.

Results: The LES and LDM runs were successfully executed for free and forced convection in the Labrador Sea. Conclusions can be drawn with respect to the bias and efficiency of isobaric and Lagrangian floats, and fixed moorings. We have found that LES of ocean drifters can be used to correct biases for isobaric drifter heat fluxes. These results are being used to guide and interpret float experiments.

Significance: Numerical simulation of nonhydrostatic ocean convection by LES enables realistic simulation of the response of drifters, buoys, chemical tracers, mines, and drifting organisms in the open ocean and in the nearshore environment.

JWCO: Joint Readiness and Logistics



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Specification of the Spatial Distribution of Water Vapor Using Visible-Band Geostationary Satellite Data

G.D. Modica and A.E. Lipton, "Mesoscale Assimilation of Visible Satellite Data: Modeling Cloud Cover Effects on Convection Destabilization Patterns," Preprints, 15th Conference on Weather Analysis and Forecasting, Norfolk, VA, American Meteorological Society, pp. 32-35, 1996.

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Signal/Image Processing

Signal and Image Processing (SIP) techniques are used throughout the DoD to extract useful information, such as target detection, tracking, imaging, and identification, from raw sensor signals. Signal and image processing spans from the development and simulation of new concepts, to their real-time implementation on ruggedized systems suitable for field deployment. The rapid advance of embedded HPC technology allows low-cost, scalable, programmable systems to replace the expensive point solutions previously required to meet the needs of high performance military systems.

The first two success stories apply HPC technology to challenges of advanced radars. In the first case, high-resolution imaging is sped up an order of magnitude. In the second case, a space-time adaptive processing technique is used for clutter/jammer suppression under both throughput and latency constraints. The next two success stories tackle computational problems associated with active and passive sonar. The adaptive beamforming techniques for sonar, similar to those of radar, can be refined with the help of HPC. In the fourth story, new decomposition methods for sparse, rank-deficient matrices delivering tenfold improvements over existing library functions are successfully moved to HPC. The fifth and sixth success stories apply HPC to real-time image processing. At White Sands Missile Range, New Mexico, a van-mounted TMC CM-500 sorts and classifies objects in real time to support kill assessments from missile intercepts. At the Air Force Research Laboratory, real-time imagery from new infrared cameras is being fused with LADAR information in real time to improve missile tracking. The final success story offers an enhanced environment to support the rapid development of parallel HPC codes for future success stories. By moving the scalable programming environment to a portable version available at several HPCMP centers, signal and image processing researchers can both shorten and simplify processes for implementing and fielding their ideas in HPC-based signal/image processing systems.

Richard W. Linderman
Air Force Research Laboratory
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CTA Leader for SIP

High-Speed Radar Imaging for Airborne Target Identification

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Space and Naval Warfare Systems Center, San Diego, CA

HPC Computer Resource: Convex Exemplar SPP-1600 [SSCSD DC]

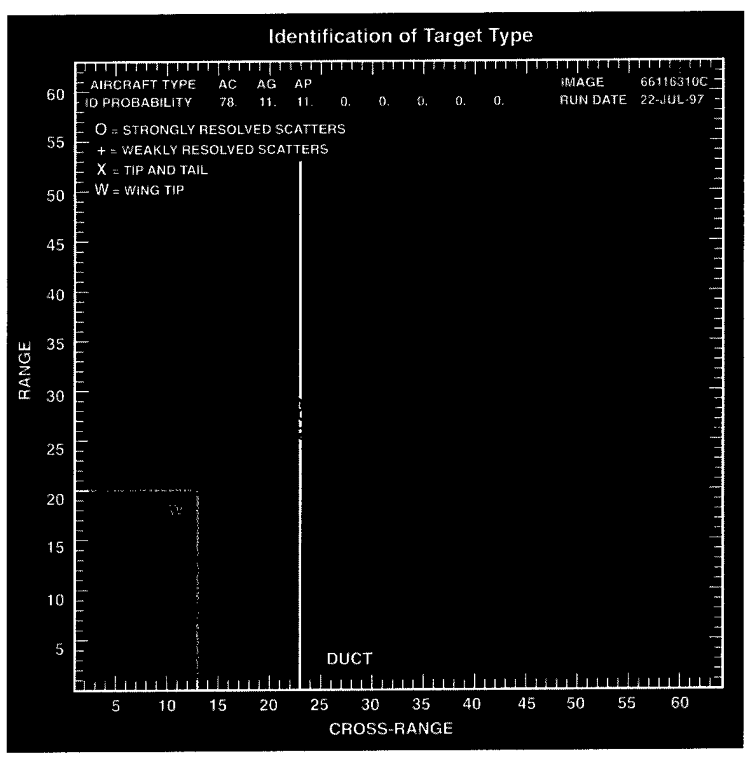
Research Objective: To make the Noncooperative Airborne Target Identification Code (NATRIC) portable and to obtain a quick turnaround to foster further research and analysis in the radar algorithm-development community. NATRIC is a large suite of computationally intensive software that has been made available by the Office of Naval Research to government researchers and contractors for further studies. It is the cumulative result of more than a decade of research to solve difficult signal and image processing problems in inverse synthetic aperture radar (ISAR). The suite, however, takes an average of one hour on a Sun SPARCstation 10 to process one second of data.

Methodology: The Convex Exemplar SPP-1600 was used for two reasons. First, it is a state-of-the-art platform of scalable shared memory parallel computers with full cache coherence supporting both message passing and symmetric multiprocessing programming. Second, NATRIC's graphical presentations, often commingled with computation, are performed by NCAR Graphics, which is available for the Exemplar. Therefore, no additional effort for code modification (to separate graphics from computation) and porting (graphics to another package) was required. For portability and for being immediately useful to radar researchers, NATRIC was initially ported to Khoros, a visual programming environment. For processing speedup, the compute-intensive components of NATRIC were parallelized using the message-passing interface (MPI).

Results: Turnaround in processing time for one second of data was shortened from 60 minutes on a Sun SPARCstation 10 to between 5 and 6 minutes on the Convex Exemplar SPP-1600, depending on the data segment, when using between two to six processors. (This includes the run-time of one component that needed to be processed on a uniprocessor SPARCstation.)

Significance: Experiences by U.S. Naval forces in the Persian Gulf War and previously in the Vincennes disaster brought into focus a serious surveillance problem — namely, long-range, noncooperative target recognition for air-threat identification. Radar imaging algorithms can solve this problem; however, they are extremely computationally intensive. This reduction in turnaround computation time from 60 minutes to 5 minutes will allow DoD scientists to experiment with various algorithmic nuances and see the results interactively instead of in an overnight batch-processing mode. This should provide a dramatic increase in productivity, which will result in improved algorithms and ultimately in improved air-threat identification systems.

JWCO: Combat Identification



A range/cross-range plot from NATRIC processing with a superimposed outline of the NATRIC-estimated most-probable target

Design, Implementation, and Evaluation of a Parallel-Pipelined STAP on Parallel Computers

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W.K. Liao, P. Varshney, and D. Weiner
Syracuse University, Syracuse, NY
R. Linderman and M. Linderman
Air Force Research Laboratory, Rome, NY

HPC Computer Resource: Intel Paragon [AFRL DC]

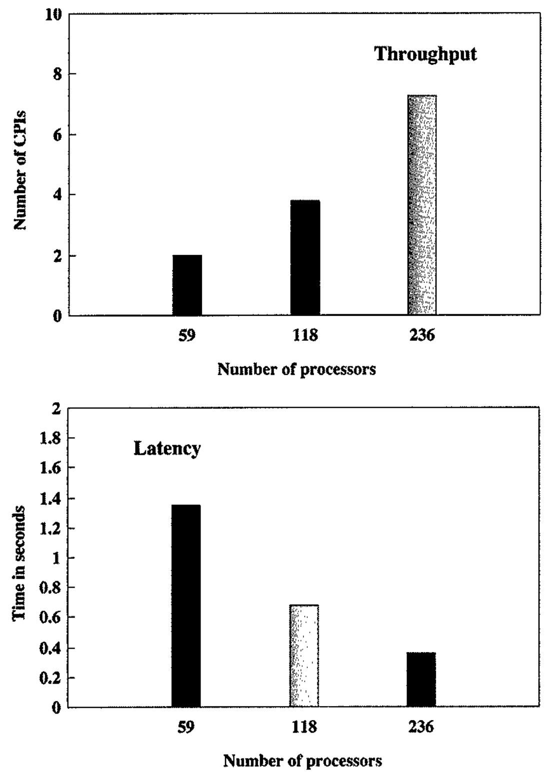
Research Objective: To design, implement, and evaluate computationally intensive signal processing applications on high-performance parallel embedded systems. As part of this project, we have developed and deployed techniques for parallelization, task mapping and allocation, parallel-pipelined communication, and data redistribution for applications consisting of several tasks. Another important goal of this project is to achieve a balance of throughput and latency through optimal use of the finite computational resources.

Methodology: We have completed an implementation of the PRI-Staggered Space-Time Adaptive Processing (STAP) application. This STAP algorithm involves Doppler filter processing, weight computation, beamforming, pulse compression, and constant false alarm rate (CFAR) processing. We designed a parallel-pipelined computation model for this STAP algorithm, as shown in the figure below. The pipeline is a collection of tasks, each of which is parallelized. This implementation is portable across different parallel machines.

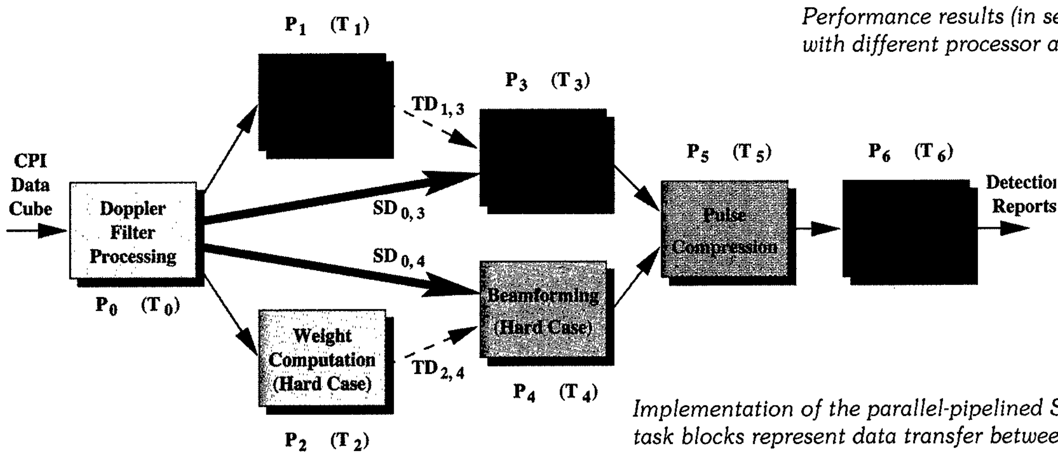
Results: In initial results, we have obtained a latency of 362 ms with a throughput of 7.3 inputs per second for the entire application (right-hand figure). This clearly demonstrates the scalability of our approach not only for individual tasks but also for the entire application in terms of both latency and throughput. Many new optimizations are currently being designed and will be incorporated in the future.

Significance: This parallelized STAP application is one of the few used in the DoD (Rome Laboratory has successfully implemented this STAP algorithm on-board an airborne platform) and is also among the most computationally intensive signal processing algorithms due to its complex data and communication patterns. Our project has demonstrated that these techniques are important and that high performance parallel computers provide significant performance benefits for such applications.

JWCO: Combat Identification, Electronic Combat



Performance results (in seconds) for three cases with different processor assignments



Implementation of the parallel-pipelined STAP. Arrows connecting task blocks represent data transfer between tasks.

Quantification of Active Sonar Adaptive Beamformer Performance

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T. Barnard and J. Smigel
Lockheed-Martin, Syracuse, NY

HPC Computer Resource: Intel Paragon [SSCSD DC]

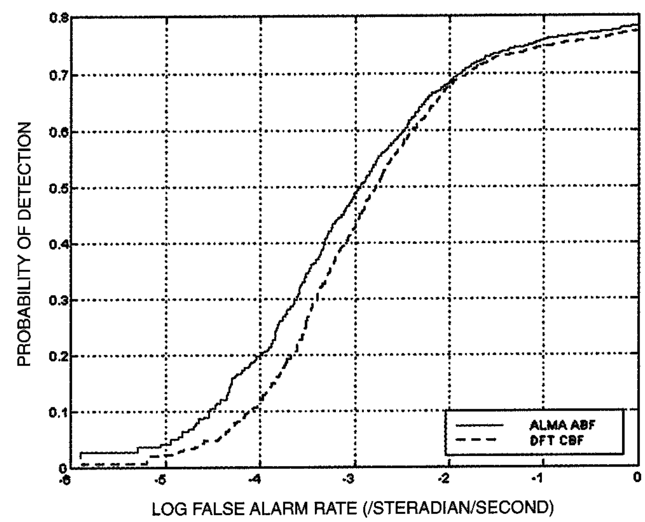
Research Objective: To significantly improve quantification of performance gains of adaptive spatial processing in sonar and radar systems. Adaptive spatial processing has provided significant advancements in interference rejection in sonar and radar systems. However, quantifying those gains is difficult because performance is scenario-dependent and both signal and interference rejection can occur. A method of performance (MOP) must take into account detection performance as well as interference reduction. Robust, statistical performance measurement is further complicated by the sparse set of target detection opportunities in active surveillance sonar systems and the computationally intensive nature of the algorithms.

Methodology: A functional, scalable testbed for an active surveillance sonar system was used to process a large recorded data set that was augmented with artificial target returns to provide a significant number of detection opportunities and exact knowledge of ground truth. Adaptive beamformer (ABF) and conventional beamformer (CBF) modules were switched to provide direct comparison of detection and interference rejection. The top figure shows the receiver operating characteristic curve for a typical run involving 125 transmissions and 1250 targets. The data set spanned 2 hours of data collection and traversed 18 kilometers. The overall performance improvement was computed as the ratio of the ABF to CBF false alarm rates averaged over all detection probabilities. The bottom figure shows the false alarm rate reduction over a range of two adaptive processing parameters. The complete study involved six parameters.

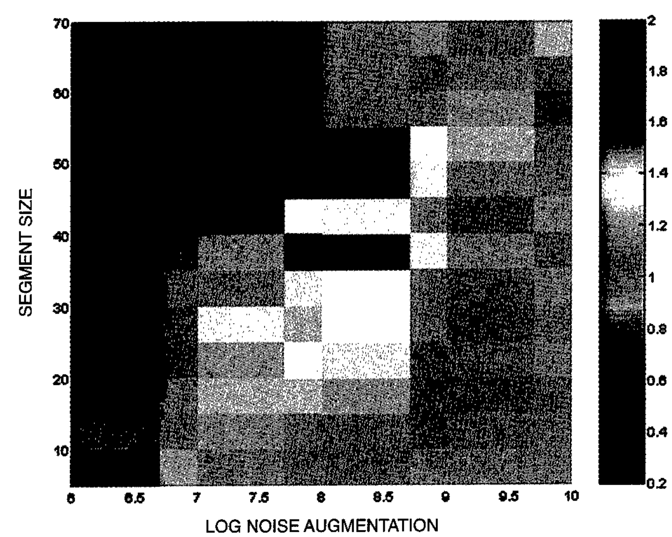
Results: Robust, statistical performance improvement over a large data set was demonstrated for active ABF. The evaluation was done in a system context providing direct, meaningful comparisons for active surveillance sonar system designers. The use of the scalable programming environment, a scalable signal-processing application programming interface, allowed throughputs twice as fast as real time for ABF and seven times faster than real time for CBF and significantly reduced development time.

Significance: The application of ABF to active sonar surveillance will improve detection and classification of difficult threats in highly cluttered littoral warfare scenarios.

JWCO: Electronic Combat



Typical receiver operating characteristic curve comparing ABF performance with that of a CBF



Average false alarm rate reduction of adaptive vs conventional beamforming for two adaptive processing parameters

Bistatic Target Strength Prediction from Limited Data

A.K. Kevorkian, D. Barach, and G.W. Benthien
Space and Naval Warfare Systems Center, San Diego, CA

HPC Computer Resource: Convex Exemplar SPP-1000 [SSCSD DC]

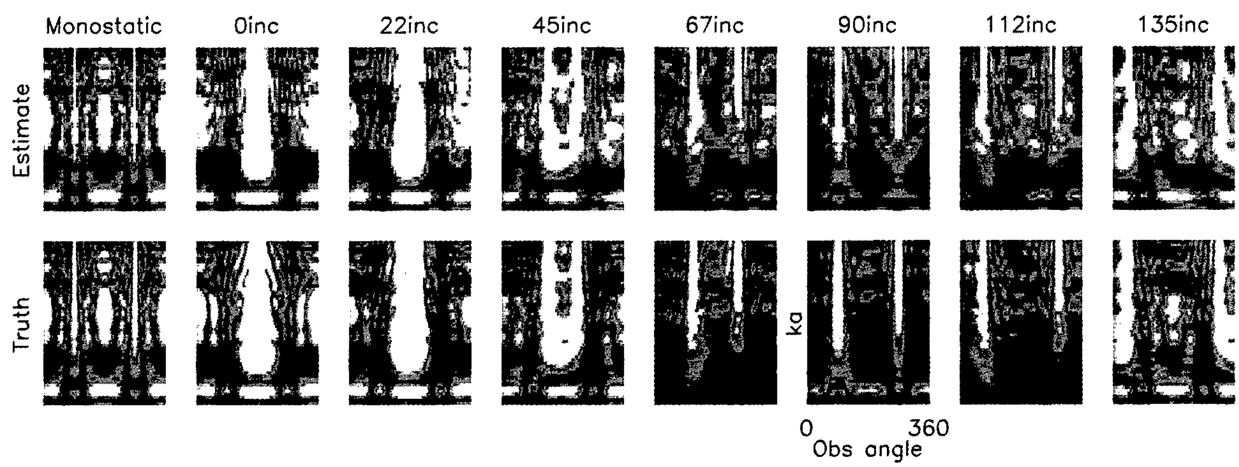
Research Objective: To develop a fast parallel algorithm that enables the extension of the frequency range relevant to bistatic target strength prediction to regions of greater interest to the Navy. Knowledge of bistatic target strength is of increasing importance in sonar systems. Full-scale measurements of monostatic target strength are expensive and difficult and become impractical for general bistatic geometries. A numerical model developed by Schenk, Benthien, and Barach uses measured monostatic and limited bistatic data to estimate the surface field and propagate it to the farfield for full bistatic geometries. The solution of this model by available conventional algorithms is time consuming, and this severely limits the frequency range of applicability. Existing data sets cannot be fully exploited using present solution techniques.

Methodology: The most compute-intensive component in the bistatic target strength model involves the least-squares solution of large, sparse, rank-deficient, overdetermined matrices. Available conventional algorithms, such as those contained in the linear algebra package LAPACK, deal with the rank deficiency but take no advantage of the sparsity inherent in these models. Therefore, they are very time consuming, and this makes the method impractical for existing data sets. We developed a new complete orthogonal factorization method that takes full advantage of the structure and numerical properties in sparse, rank-deficient, overdetermined systems of the type arising in the bistatic target strength prediction models. The sparse overdetermined matrices in these models belong to a class called row-bordered block diagonal matrices.

Results: By applying this new decomposition method to a range of highly ill-conditioned, rank-deficient, bistatic, target strength prediction models, we have obtained a five- to sevenfold improvement over the compute time required by LAPACK without exploiting any parallelism. By exploiting parallelism in one key part of our method, we have obtained improvements over LAPACK from nine- to fifteenfold. Further speedups can be realized by exploiting parallelism in all parts of the new method.

Significance: Since the size of the problem increases rapidly with frequency, the speedups gained from the new method will enable the frequency range in bistatic target strength prediction models to be extended to regions of greater interest to the Navy.

JWCO: Information Superiority



Comparison of estimated and true monostatic and bistatic target strength surfaces. The color bar maps target strength in dB to each particular color.

Real-Time Sorting and Classification of Unresolved Objects

D.H. Marlin and J.G. Ambrose
U.S. Army White Sands Missile Range, NM

HPC Computer Resource: TMC CM-500 [WSMR DC]

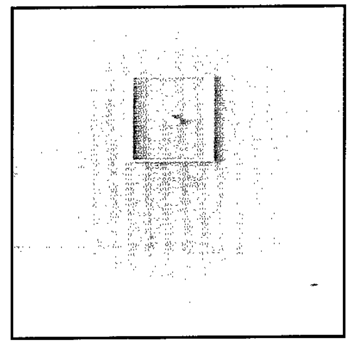
Research Objective: To enhance test and evaluation of tactical and strategic weapon systems by improving the ability to sort and classify objects in real time, especially as a sparse object field discontinuously evolves into a dispersed and cluttered field. In a tactical setting, the dispense of submunitions from a subsonic missile carrier creates such an object field. A strategic application involves assessing a kill from the debris field generated in a missile-to-missile intercept (real-time battle damage assessment). Both applications are fundamentally the same and require a significant peak real-time computational capability. A binary classification scheme is fully implemented on a modified CM-500 to achieve very low system latencies.

Methodology: A significant adaptation of hardware, firmware, and the development of a real-time kernel was carried out on a van-mounted CM-500. The CM-500, a prototype evolved from a CM-5E, was configured to substantially increase I/O bandwidth. This yielded interprocessor broadcast times 15 times smaller than those of the CM-5E. Internal system communication latencies were minimized by generating independent multi-instruction cells running under separate real-time operating systems on each of the two partition managers (PM). Each PM controls a subset of the available processing nodes. Interprocessor communications are constrained by the node assignments made to each PM, thus limiting the maximum interprocess broadcast time. PM-to-PM data broadcasts are handled by a PM message-passing configuration. All communication that must be directed to a process running in a separate PM travels through low-level message-passing protocols.

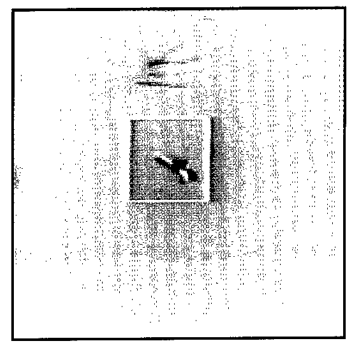
Results: An automated vision module (AVM) algorithm that performs sorting and classifying was developed. The AVM is specifically designed for the real-time architecture discussed above. AVM analyzes the images by processing video feeds generated from a pair of IR focal plane starring arrays. The real-time AVM analysis consists of polling for an event, cluster tracking, kinematics and signature prediction, and application of the blob function. The combination of multiple look angles from each of two PMs completes the real-time sorting and classifying in less than two video frames of total accumulated system latency. The kinematics prediction is histogram based, while the signature predictor relies on the ratio of image content in two separate spectral bands. The blob function is object-sized and shape-based for cases where the objects to be tracked are resolved. The two PM processes outlined here are undergoing scale-up to ten simultaneous look angles with dedicated I/O.

Significance: This development was applied to assess the performance of high-speed interceptors and tactical deep strike weapons undergoing developmental testing. Programs such as ATACMS/BAT, THAAD, and SM-3 are actively adapting HPC computing hardware while developing code for real-time applications. What has emerged is a significant capability to provide a real-time sensor fused data source for battle damage assessment.

JWCO: Information Superiority, Electronic Combat



(a)



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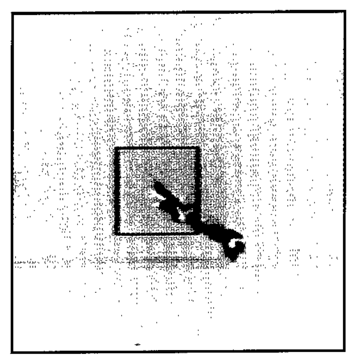

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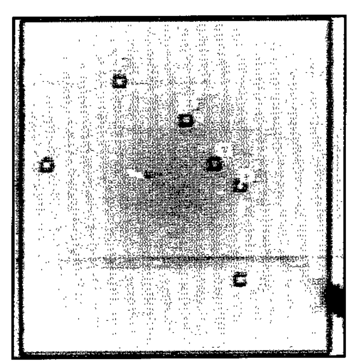

(d)

All three states of the AAVM are represented in this figure. In (a) the AAVM is in ACQUIRE state having located and identified the primary carrier; in (b) a dispense event has begun, and the AAVM is in the POLL state looking for dispense; in (c) the AAVM has recognized dispense and has entered CLUSTER state to acquire submunitions; finally, in (d) the AAVM has acquired multiple submunitions, which are being qualified by behavioral kinematics models.

Real-Time Sensor Fusion Tracking

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D. Fronterhouse
Scientific Simulation, Inc. Galveston, TX
L. Gratch, G. Bright, and M. Barnell
Computer Sciences Corporation, Rome, NY

HPC Computer Resource: Intel Paragon [AFRL/ID DC]

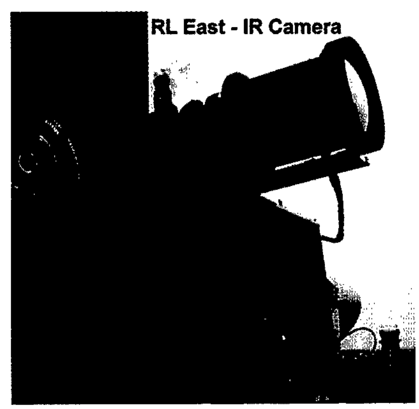
Research Objective: To develop, test, and demonstrate fusion of various sensor technologies for Theater Missile Defense. The Ballistic Missile Defense Organization initiated the Advanced Sensor Technology Program to assemble and test an existing multisensor fusion algorithm, and then evaluate its ability to acquire, track, and identify boosting and ballistic missile targets as observed from an airborne platform.

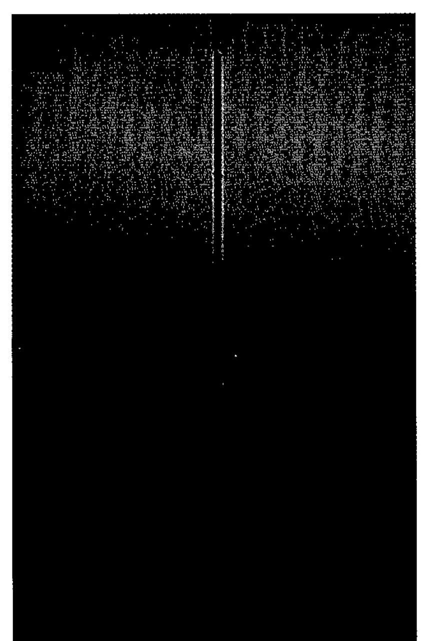
Methodology: This algorithm was implemented on the Intel Paragon and tested in real time through the use of the Scale Rocket experiments at Rome Laboratory (now the Air Force Research Laboratory). Experimental testing and demonstrations involved live representative scale rocket targets where data from multispectral sensors were fused to enhance overall detection, tracking, and target identification. Real-time processing of target detection, data correlation, precision tracking, and plume-to-hardbody handover were accomplished. A functional testbed was developed for the Intel Paragon, and the necessary communication links between the infrared (IR) and laser detection and ranging (LADAR) sensors and the Paragon processor's high performance parallel interface board were established via a fiber channel. The algorithms ran and received sensor data in real time.

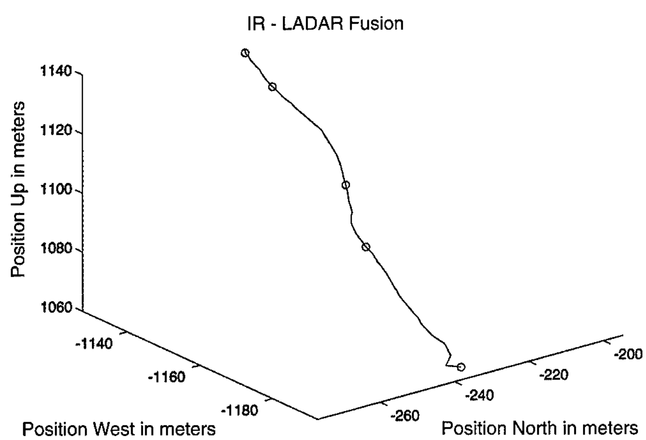
Results: This project successfully demonstrated real-time communication and sensor fusion tracking of a scale rocket.

Significance: This project was the first live demonstration of real-time closed-loop tracking and sensor fusion to link two IR sensors (a tracking radar and a LADAR) to a high performance computer.

JWCO: Joint Theater Missile Defense







The RL East-IR Camera was used to track the scale rocket in the 3 to 5 μm band. The scale rockets are 1 m long by 6 cm in diameter with a motor burn time of 9.8 seconds. The data were fed to the high performance computer, and the curve shows that sensor fusion was accomplished; the position track file is shown in the coordinate system of Up, West, and North.

Scalable Prototyping of Embedded Signal Processing Systems

P. Partow and D.M. Cottel
Space and Naval Warfare Systems Center, San Diego, CA

HPC Computer Resource: Intel Paragon [SSCSD DC]

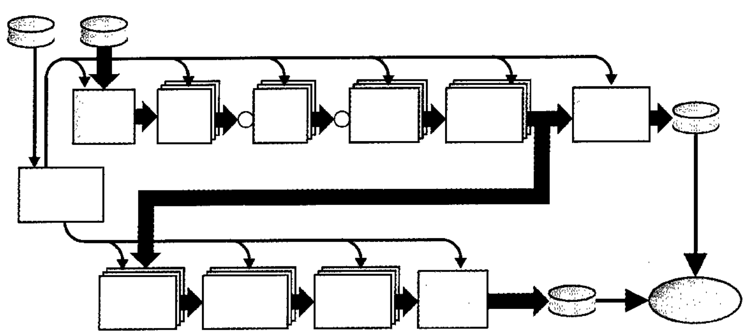
Research Objective: To develop a portable version of the SSCSD Scalable Programming Environment (SPE) and to provide and support versions for various HPC systems and for networks of workstations. DoD embedded signal processing applications are currently developed as conventional sequential programs and then rewritten as parallel programs for a specific embedded architecture. The SPE provides a way to develop scalable, parallel signal and image processing applications that can, by simple recompilation, be ported to various HPC architectures and ultimately to embedded systems. The concepts have been proven on the Intel Paragon where the SPE is in production use.

Methodology: The SPE is intended to be used for real-time signal processing and so has been implemented as an efficient environment for building applications in a modular, flexible, scalable manner. It handles the myriad complicated details of scalable parallelism so that programmers can concentrate on signal processing issues. The SPE has been successful not only in providing transparent scalability for users, but also in encouraging good software engineering practices such as modularity, well-defined interfaces, and rapid prototyping of parallel programs. The SPE was originally developed for a specific project funded by the Office of Naval Research, using the Intel Paragon at the SSCSD DC. Since that time, the message-passing interface (MPI) standard has become widely adopted as a low-level method of making parallel message passing programs portable to multiple HPC platforms. By taking advantage of the portability of MPI, the SPE has been made much more portable so that signal processing applications may be quickly ported to new hardware architectures.

Results: Under the DoD HPC Modernization Program, with very little change to the user-visible programming interface, the SPE was redesigned and reimplemented to use MPI-1 for communication between processes. Initial beta test versions of the SPE have been distributed to potential users of Windows NT, Sun Solaris, and Silicon Graphics IRIX systems. Projects involving synthetic aperture radar (SAR) at SSCSD, automatic target recognition (ATR) at AFRL, and image compression and ATR at the Army Night Vision Laboratory are developing SPE-based scalable, parallel modules, which will be interconnected in a planned tri-service interoperability demonstration. SSCSD and Sanders are collaborating to develop an implementation of the SPE for the Sanders Embedded High Performance Scalable Computing System. Khoral Research, Inc., the developers of Khoros, is considering ways of incorporating SPE technology into the Advanced Khoros project currently funded by the Defense Advanced Research Projects Agency (DARPA).

Significance: With availability on a wide variety of platforms, the SPE has the potential to be the foundation on which parallel, scalable software modules can be provided to the signal and image processing community. Because of the SPE's support for modular programming, the various modules can be freely interconnected in much the style of Khoros. The resulting applications can be directly ported from workstations to HPC systems, and to any embedded system for which the SPE has been implemented.

JWCO: Joint Readiness and Logistics



Functional and data flow diagram of an operational active sonar processor implemented as a parallel, scalable HPC program. The application will run on an arbitrary number of nodes of the Intel Paragon.

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Design, Implementation, and Evaluation of a Parallel-Pipelined STAP on Parallel Computers

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Bistatic Target Strength Prediction from Limited Data

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Forces Modeling and Simulation/C4I

Forces Modeling and Simulation/Command, Control, Communications, Computers and Intelligence (FMS/C4I) focuses on research that uses high performance computing to provide dominant battlespace knowledge. This area is directly impacted by the High Level Architecture developed by the Defense Modeling and Simulation Office and the Joint Technical Architecture developed by the Defense Information Systems Agency. Adapting and enabling the use of parallel computing for these application domains is the focus of this CTA. The three success stories in this section show the complexity of this application domain. It is dominated by large, complex systems rather than by small, classical supercomputing codes. A combination of parallel processing, object-oriented programming, and real-time interaction is characteristic of this domain. The first success story examines the implementation of Enhanced Modular Semi-Automated Forces (E-ModSAF), one of the most highly used simulation systems in DoD, in the new shared-memory architecture machines that are becoming very popular in the high performance computing world. The second success story addresses the combination of faster than real-time simulation for a Joint Theater Missile Defense simulation application. The third provides a capability to perform Joint Strike Fighter Mission Planning.

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San Diego, CA
CTA Leader for FMS/C4I

Enhanced ModSAF Architecture for Higher Fidelity Warfighter Training

J.G. Steele, M.D. Roberts, J.McCutcheon, and J.W. Willcox III
Space and Missile Defense Command, Huntsville, AL

HPC Computer Resource: SGI Origin 2000 [SMDC DC]

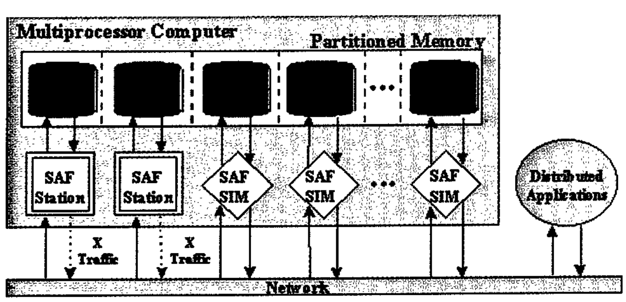
Research Objective: To modify a ground force modeling simulation to use shared memory on multiple processor high performance computers for the Enhanced Modular Semi-automated Forces (E-ModSAF) project. By using shared memory and centralized process control, redundant network traffic and database overhead are eliminated, providing significant and scalable performance increases per processor. These performance increases allow for the modeling of more complex scenarios involving larger numbers of entities thereby enabling higher fidelity warfighter training.

Methodology: The E-ModSAF architecture leverages the existing ModSAF design while providing three additional components: protocol data unit (PDU) Reader, PDU Writer, and an Executive. The PDU Reader reads and processes all network messages into a single shared-state database used by all SAFSims and SAFStations. The PDU Writer writes PDUs to the network. The Executive controls and monitors all E-ModSAF processes via a user-friendly graphical user interface. The Executive provides fault tolerance to processes and dynamic load balancing, allowing maximum usage of available HPC resources.

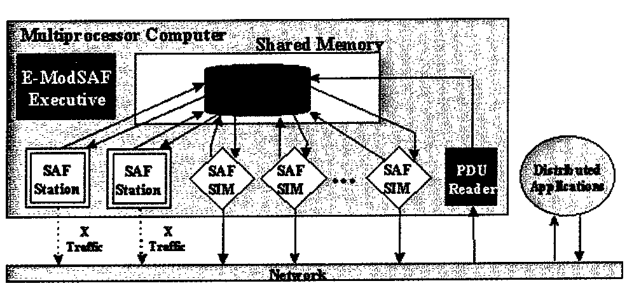
Results: The E-ModSAF effort has proceeded successfully through the Requirements/Proof-of-Concept Development phase and is currently in the Design/Prototype Development phase. The higher fidelity modeling provided by E-ModSAF supports the enhanced simulation for training capability of the Joint Readiness and Logistics joint warfighting capability objective.

Significance: By enabling larger and more complex scenarios involving significantly higher numbers of entities, E-ModSAF allows the warfighter to participate in more comprehensive training exercises. Similarly, analysis capabilities are increased, thereby supporting enhanced readiness and improvements to logistics for joint and combined operations. The technologies demonstrated as part of the E-ModSAF project can be applied to other advanced simulations allowing state-of-the-art HPC resources to be optimally used to support the warfighter. By increasing the performance of advanced simulations on HPC resources, the hardware cost-per-modeled-entity is also reduced.

JWCO: Joint Readiness and Logistics



Existing ModSAF for Distributed Memory Multiprocessors
- *Independent/cooperating control*
- *Separate entity state databases*
- *High entity interaction overhead*
- *Database redundancy and coherence overheads*



Enhanced-ModSAF for Shared Memory Multiprocessors
- *Centralized control*
- *Single shared entity state databases*
- *Efficient entity interaction*
- *Simplified load balancing and fault tolerance*

Joint Theater Missile Defense

K. Barry and D. Jackson
Naval Air Warfare Center Aircraft Division, Patuxent River, MD

HPC Computer Resources: SGI PCA [NAWCAD DC]

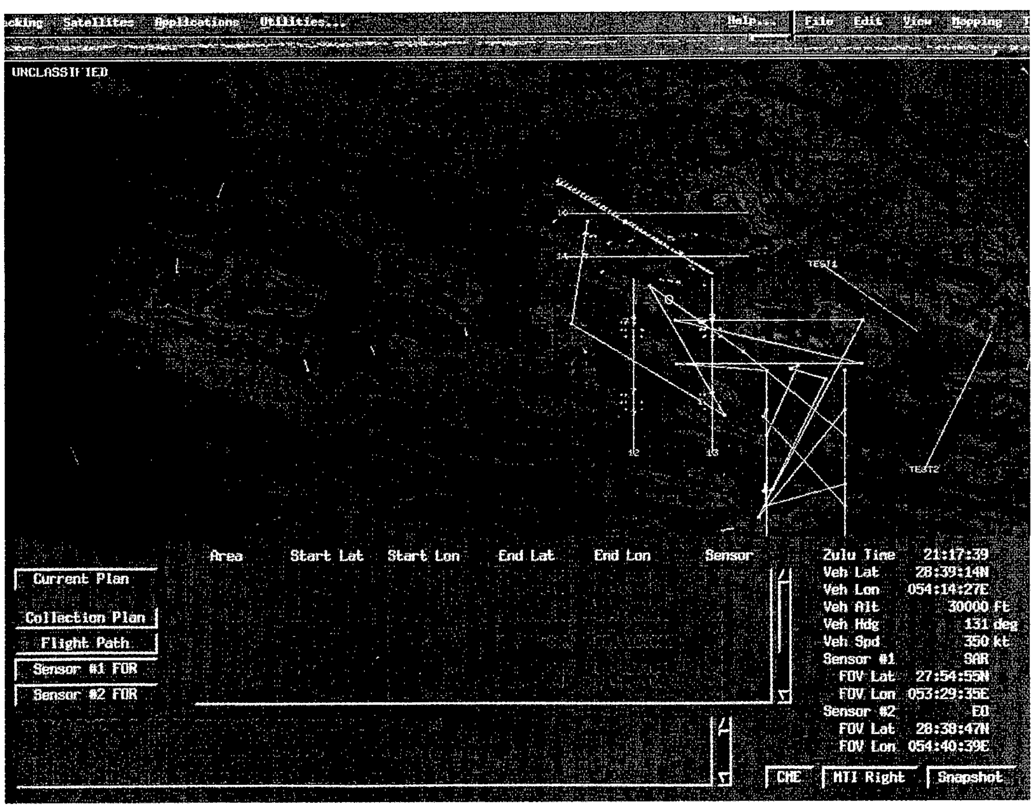
Research Objective: To investigate methods and technologies that assess the capabilities available to the Commanders in Chief to integrate near-term systems during joint theater missile defense attack operations.

Methodology: The Joint Theater Missile Defense Attack Operations Joint Test and Evaluations Program ran a real-time, mission-level, simulated warfare environment generator and four high-fidelity man-in-the-loop (MITL) flight and avionics simulators. These MITL assets used 3-D geometry processing and texture-mapped imagery at greater than real-time frame rates to model out-the-window scenes and heads-down displays. Multiple defense internet simulator interfaces, stick and throttle interactions, visuals, and flight dynamics were processed concurrently. In addition, asset data structures were passed real time via a Shared Common Random Access Memory Network (SCRAMNet) and encrypted networks to external real-time assets and remote sites, respectively.

Results: Interactive displays in the MITL simulators allowed visual and avionics clients to provide high-fidelity rendered displays of acquired targets, antiaircraft artillery/surface-to-air missile (AAA/SAM), and terrain, as well as support for general search and final acquisition modes.

Significance: These experiments addressed critical operational issues including adequacy of near-term sensors, effectiveness of near-term C^{4}I, effectiveness of attack systems, and the impact of individual systems to destroy and suppress theater missiles.

JWCO: Joint Theater Missile Defense



Global Hawk UAV synthetic aperture radar and moving target indicator sensors on one of the joint theater missile defense's (JTMD's) reconfigurable sensor ground stations. These ground stations allowed the operator to control the sensor perform C4I exercises.

Joint Strike Fighter Mission Planning

M. Piland
Naval Air Warfare Center Aircraft Division, Patuxent River, MD

HPC Computer Resource: SGI Origin2000/Onyx2 [NAWCAD DC]

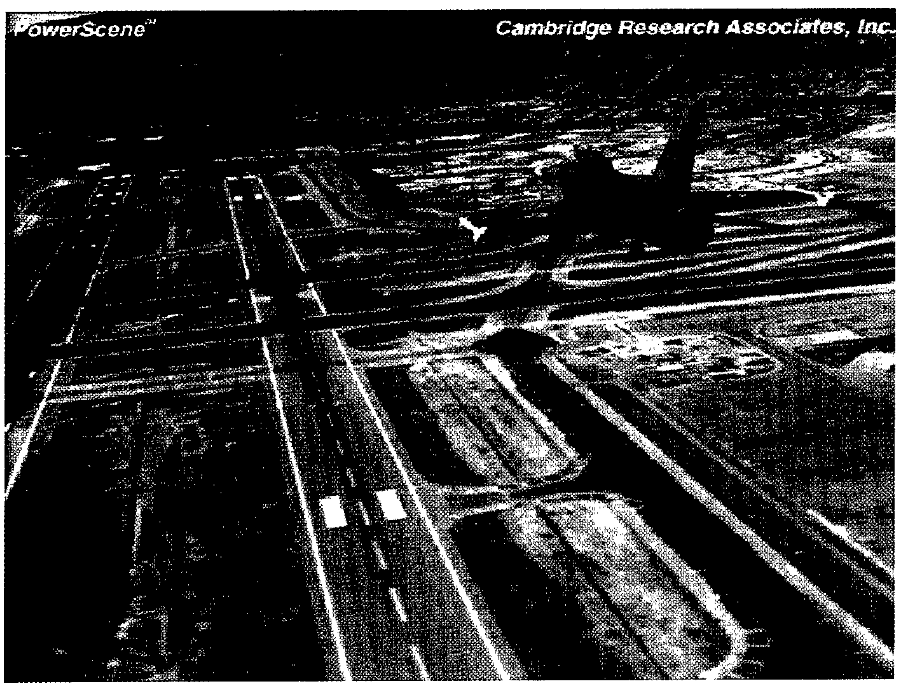
Research Objective: To create a high-fidelity war-game environment where tactical concepts can be exercised and investigated for feasibility in defining requirements.

Methodology: The Joint Strike Fighter (JSF) Program Requirements Directorate used the Cambridge Research Associates' Power Scene™ software to display high-resolution photo imagery. Terrain data mapped with satellite images and aerial photographs were rendered in real time and sent to remote Air Combat Environment Test and Evaluation Facility simulation laboratories via optically linked control systems for interactive mission feedback. Infinite Reality graphics engines were used to process a large visual database into appropriate textures and images in real time. This provided a realistic scene that was then correlated with the Air Force mission system simulation.

Results: Improved real-time rendering of Power Scene™ visual databases.

Significance: The improved performance provided the warfighters and planners a more realistic environment in which to rehearse the planned missions. This, in turn, gave the warfighters additional means to make valued judgments with respect to current JSF concepts under technical consideration.

JWCO: Precision Force



Sample Power Scene™ imagery database representative of those used by JSF during simulation exercises

Selected References

Enhanced ModSAF Architecture for Higher Fidelity Warfighter Training

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Environmental Quality Modeling and Simulation

The Environmental Quality Modeling and Simulation (EQM) computational technology area focuses the use of high performance computing in support of the Department of Defense's environmental quality management activities. As the steward for the nation with nearly 50 million acres of land, DoD has a vibrant program of environmental restoration and land management on its installations and in support of national infrastructure. EQM technology is a key component of this program.

The EQM success stories presented here are but a few examples of the use of HPC technology in environmental quality research, development, and site-specific application being conducted within DoD. The stories provide a representative flavor of the vital role HPC technology plays in enabling DoD to implement technically proficient, cost-effective environmental management. The stories provide a snapshot into the computationally intensive contaminant transport modeling and simulation that DoD performs in support of installation cleanup and conservation. The stories further depict the critical role HPC plays in the development of vastly improved subsurface modeling in heterogeneous media. Finally, these stories (and two analogous stories in the CFD section) illustrate the high potential that exists within DoD for accelerated technology development through synergism between computational technology areas.

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CTA Leader for EQM

Three-Dimensional Contaminant Transport and Fate for Surface Water

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Army Engineer Waterways Experiment Station, Vicksburg, MS

HPC Computer Resource: Cray C90, Cray T3E, SGI PCA, SGI Origin 2000, and IBM SP [CEWES MSRC]

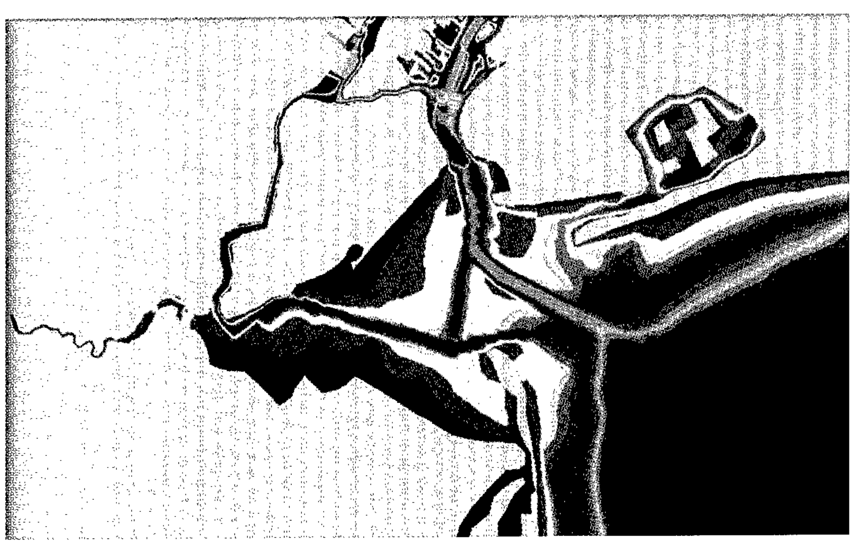
Research Objective: To develop a three-dimensional (3-D) modeling system for contaminant transport and fate in surface water that can be applied on scalable parallel computer systems.

Methodology: The focuses are on the development of a scalable software system for modeling the transport and the fate of contaminants in bodies of surface water such as lakes, rivers, bays, and estuaries. This 3-D modeling system consists of three coupled components for hydrodynamics, fine-grained sediment transport, and contaminant transport/fate that are being implemented within the surface water modeling system graphical user environment for ease of application. Software implementation is based on high-level programming languages as defined by international standards organizations such as ANSI (e.g., FORTRAN) with explicit message-passing interfaces using the message-passing interface (MPI) standard for distribution of simultaneous computational tasks while providing cross-platform portability. Additionally, C is used for the human-computer interface software. Scalability is achieved through judicious use of domain decomposition and load balancing.

Results: This project is in the second year of a four-year study. The hydrodynamic, sediment transport, and contaminant transport/fate components have been coupled and applied to the harbor-apex model for polychlorinated biphenyls (PCBs). The modeling system yields accurate results for tides, currents, suspended solids, concentrations, and PCB distributions. CH3D-SED has been parallelized for a shared memory environment using MPI and is being evaluated on various multiprocessor platforms. Work on converting the model to run in a distributed memory environment is ongoing. Work on conversion of the integrated compartment model using MPI is also underway.

Significance: Dynamic 3-D simulations of this nature are an essential part of DoD's environmental quality management activities in the areas of compliance, conservation, and cleanup. In particular, the modeling technology discussed here is used (in concert with effective monitoring) to assess and implement cost-effective pollution prevention and ecosystem restoration activities in estuaries, harbors, and other strategic waterways of importance to national defense. The scalable parallel capabilities being fielded by this CHSSI project represent the leap in 3-D contaminant fate/transport modeling needed to meet DoD's present and future environmental quality management needs.

JWCO: Joint Readiness and Logistics, Chemical/Biological Warfare Defense and Protection



Bathymetry and platform grid for New York bight and harbor

Modeling Flow and Transport in Heterogeneous Media

A.R. Carrillo, S.E. Howington, J.F. Peters, and F.T. Tracy

Army Engineer Waterways Experiment Station, Vicksburg, MS

S.G. Smith and C.S. Woodward

Lawrence Livermore National Laboratory, Livermore, CA

HPC Computer Resource: Cray T3E and IBM SP [CEWES MSRC]

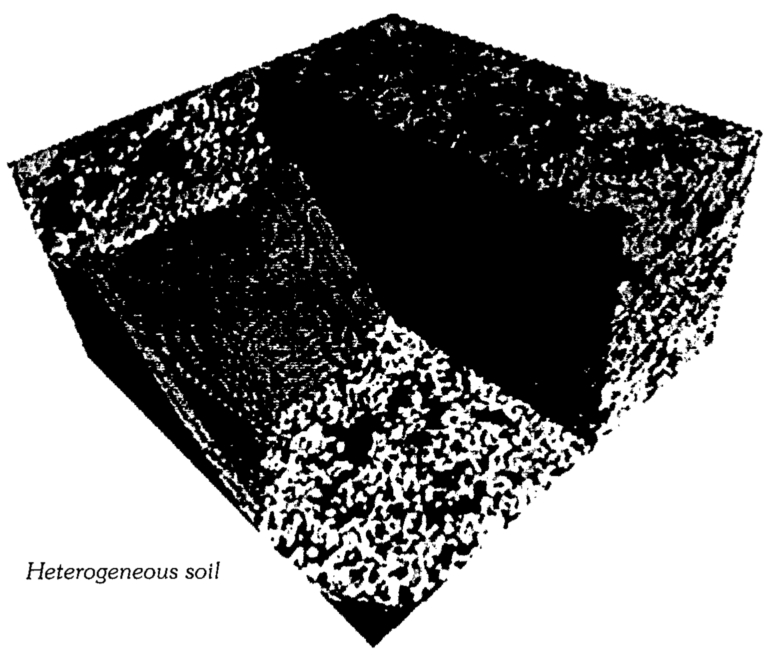
Research Objective: To develop and implement a highly resolved (10s of millions of computational nodes) continuum model for subsurface flow and transport whose statistical results will form the constitutive basis of a new class of more economical subsurface particle models with memory.

Methodology: PARFLOW, a three-dimensional, finite-difference model with integrated capabilities to statistically represent subsurface heterogeneities, is the primary tool for high-resolution continuum modeling being conducted in this investigation. A particle model, based on correlated random-walk transport techniques, is also being executed in concert with PARFLOW.

Results: Initial correlated random-walk transport calculations demonstrated that dispersivity, a primary process whose parameterization is key to accurate subsurface modeling, may be simulated more efficiently with the products of this project than with highly resolved continuum models. Implementation of the PARFLOW model on the Cray T3E and IBM SP was completed, thereby allowing expanded investigation of the validity of this hypothesis. Rigorous verification of this hypothesis would not be computationally possible without DoD scalable HPC resources.

Significance: These results advance the state-of-the-art of modeling flow and transport in heterogeneous media. This improvement of modeling capability will result in more economical and better cleanups, thus giving the warfighter improved facilities and more resources for direct support.

JWCO: Joint Readiness and Logistics



Heterogeneous soil

Coupled Structured-Unstructured Flow Simulation

R.S. Bernard, R.C. Berger, R.L. Stockstill, and A.K. Stagg
Army Engineer Waterways Experiment Station, Vicksburg, MS

HPC Computer Resource: Cray C90 and T3E [CEWES MSRC]

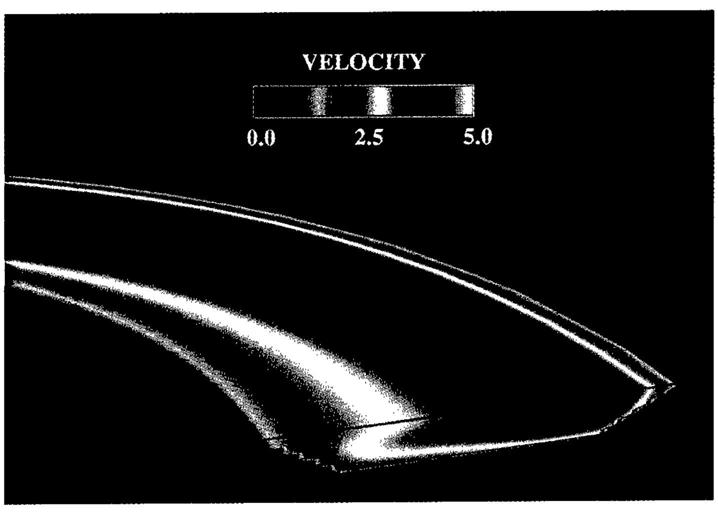
Research Objective: To implement combinations of structured and unstructured grid numerical solutions techniques for the three-dimensional, incompressible Navier-Stokes equations and associated multiconstituent transport equations, in a scalable computational framework for solving free-surface flow problems that arise from environmental concerns associated with military activities.

Methodology: In computational physics and engineering, sequentially ordered (structured) grids facilitate rapid calculation at the expense of geometric flexibility, while nonsequential (unstructured) grids offer unlimited geometric flexibility with lesser speed. By using these two types of grids simultaneously for different regions of the same flow problem, however, one can achieve the best of both worlds. Specifically, unstructured grids can be used selectively near irregular boundaries, with structured grids covering the rest of the computational domain. Moreover, the coupled implementation of structured and unstructured flow-simulation schemes lends itself naturally to parallel processing.

Results: Structured and unstructured flow-solvers have now been successfully developed and tested separately for scalability and verisimilitude on a variety of benchmark flow problems. Static and dynamic grid interfaces are currently under development that will couple the two flow-solvers in a single parallel framework. Unstructured components will reside on one set of processors, and structured components will occupy another, with message passing used to convey information back and forth between the two.

Significance: The effects of DoD activities on the ecosystems within and adjacent to military installations are a prime concern. Advanced environmental quality modeling and simulation technologies are needed to allow DoD to implement sound management strategies for these ecosystems. Certain DoD activities, such as the movement of aircraft carriers into and out of port or training on the landscape, require simulation of coupled hydrodynamic and hydrologic processes, which greatly tax current simulation techniques. The project described here will provide DoD with an expedient, economical technique to predict the effects of military operations in the aquatic-terrestrial environment.

JWCO: Joint Readiness and Logistics



Velocities computed in a curved trapezoidal channel

History-Dependent Random-Walk Simulation of Transport Through Porous Media

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Army Engineer Waterways Experiment Station, Vicksburg, MS
R.S. Maier
Army High Performance Computing Research Center, Minneapolis, MN

HPC Computer Resource: TMC CM-5 [AHPCRC DC]

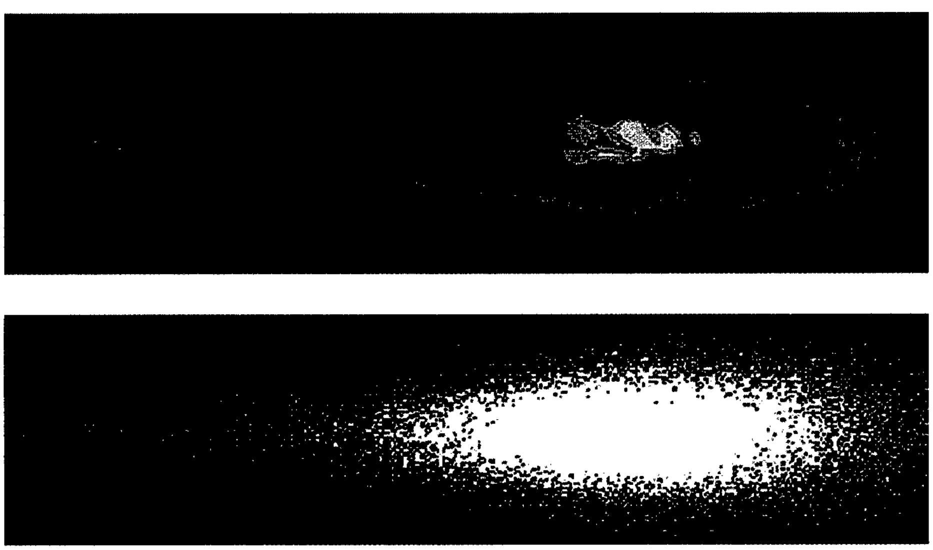
Research Objective: To make fundamental improvements in modeling dispersive contaminant transport in natural heterogeneous media by replacing highly resolved numerical simulations that describe random permeability fields explicitly with an equivalent statistical flow field. Highly resolved flow models severely tax HPC resources and limit the number of processes that can be included in the model.

Methodology: Statistics for flow velocity are obtained from highly resolved porous media simulations. These statistics are used to establish general relationships between random components of velocity and dispersion. Once the statistical laws for dispersion are established, future simulations can be performed without recourse to highly resolved flow fields. The mean velocity component is obtained from a flow simulation with minimal resolution. The random velocity component is generated as a sequence of correlated random numbers.

Results: Velocity statistics for flow through porous media were shown to display scale effects that can be expressed as a history dependence. A particle tracking analysis, derived from a standard random-walk model, was endowed with the history-dependent statistical representation of velocity. The procedure is ideally suited for parallel transport calculations in engineering-scale codes. Computer simulations showed that the mean flow fields do not require highly resolved media. Because dispersion is driven by deviations from the mean flow, a more economical computation for dispersion may be possible, provided the statistics for flow velocity deviations can be developed.

Significance: DoD is responsible for nearly 10,000 active military installations and over 6,200 formerly used installations that require environmental remediation. The costs of cleaning up these sites is estimated to range between $35 to $100 billion. Savings on the order of 10 to 20% of the costs of cleanup may be possible through implementation of these improved subsurface modeling techniques that more accurately account for the effects of subsurface heterogeneity.

JWCO: Joint Readiness and Logistics



Correlated random-walk transport computations (top) efficiently produce pre-asymptotic dispersion behavior also seen in high-resolution flow and transport simulation (bottom).

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History-Dependent Random-Walk Simulation of Transport Through Porous Media

J.F. Peters and S.E. Howington, "Pre-Asymptotic Transport Through Porous Media," in *Next Generation Environmental Models: Computational Methods*, edited by G. Delic and M.F. Wheeler, Philadelphia, PA, pp. 271-280, SIAM Books, One Volume, (1997).

J.F. Peters, S.E. Howington, and R.S. Maier, "Network Models for Field-Scale Analysis of Conservative Contaminant Transport," Presented at the Fourth SIAM Conference on Mathematical and Computational Issues in the Geosciences, Albuquerque, NM, June 16-19, 1997.

Computational Electronics and Nanoelectronics

In the Computational Electronics and Nanoelectronics (CEN) computational technology area, advanced computational methods are being used to model and simulate complex electronics for communications, command, control, electronic warfare, sensing, and related applications. Scalable software is being developed to enable efficient predictive design and efficient numerical modeling and simulation of complex electronic devices, large-scale integrated circuits, networks, and systems. The use of high performance computing assets enables the DoD electronics community to solve complex problems, explore new concepts, gain insight and improved understanding of the underlying physics, perform virtual prototyping, and test new ideas. Scalable software tools enable higher accuracy and/or increased size/complexity for such analyses.

The following examples are only a sample of numerous efforts that support a spectrum of mission requirements and demonstrate the pervasiveness and significance of electronics in DoD systems. The first success story involves a linearly scalable parallel electromagnetic solver applied to high-frequency antenna and circuit design. This effort demonstrates significant improvement in algorithms to design and optimize complex electronic structures such as integrated patch array antennas. The approach uses a wavelet-based method of moments and a tetrahedral finite-element method to efficiently handle and accelerate the analysis of arbitrary three-dimensional structures. The second story describes steady-state analysis of nonlinear circuits using the harmonic balance method. This approach allows for circuits with widely varying time constants or significant distributed element effects. Small grain code parallelization is used to achieve improved scalability with a large number of frequencies analyzed.

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CTA Leader for CEN

Parallel Electromagnetic Solvers for High-Frequency Antenna and Circuit Design

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The University of Michigan, Ann Arbor, MI
B. Perlman
Army Research Laboratory, Ft. Monmouth, NH

HPC Computer Resource: IBM SP [MHPCC DC]

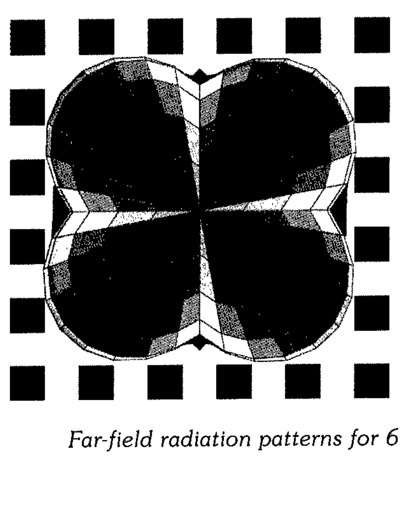
Research Objective: To develop linearly scalable parallel electromagnetic solvers for large array antenna and complicated microwave/millimeter-wave circuits that have not been successfully characterized by other means. Fast and accurate characterization of these electromagnetic structures are of critical importance for a successful DoD mission in digitizing the battlefield and developing secure communication systems.

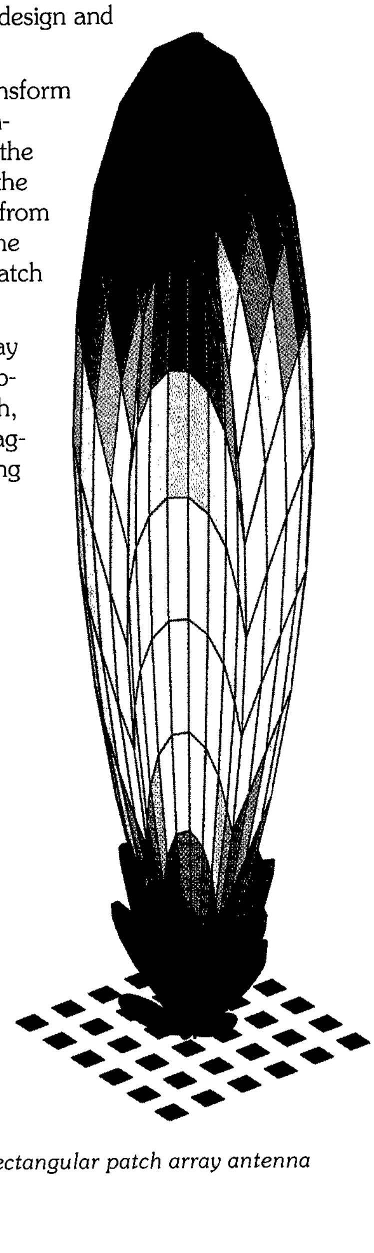
Methodology: For parallel electromagnetic tools, we have developed wavelet-based method-of-moment (MoM) and tetrahedral finite-element-method (FEM) codes for arbitrary three-dimensional (3-D) structures, and a message-passing interface (MPI) has been used for parallelization on distributed memory parallel computers. Furthermore, fast wavelet transform and thresholding techniques are applied to achieve accelerated computation of the MoM solution. The linear, scalable performance of the parallelized MoM and FEM is also investigated for real-time design and optimization of the large array antenna and high-frequency circuits.

Results: Preliminary results of the parallel impedance matrix filling and fast wavelet transform for MoM and task parallelization strategy for FEM show linearly scalable performance improvement. These truly scalable parallel MoM and FEM codes perform successfully due the minimal communication overhead between the computing nodes and are not subject to the bandwidth of the network or switches. The number of unknowns of the problem ranges from 15,000 to 20,000 in the MoM case and from 150,000 to 200,000 in the FEM case. The figures show 3-D electric field distributions at the far region from the 6 × 6 rectangular patch array antenna that are computed efficiently on parallel computers.

Significance: Design and optimization of large electromagnetic structures, such as array antennas and high-density circuits and packages, are of critical importance in the development of the advanced sensors and tactical communication systems. Through our research, we have demonstrated linearly scalable parallel strategies for various numerical electromagnetic codes and solved problems that were not possible or were extremely time consuming with conventional methods and computers.

JWCO: Electronic Combat





Far-field radiation patterns for 6 × 6 rectangular patch array antenna

Nonlinear, Frequency Domain Circuit and System Modeling

D.L. Rhodes
Army Research Laboratory, Fort Monmouth, NJ

HPC Computer Resource: SGI PCA and SGI Origin 2000 [ARL MSRC] and IBM SP [MHPCC DC]

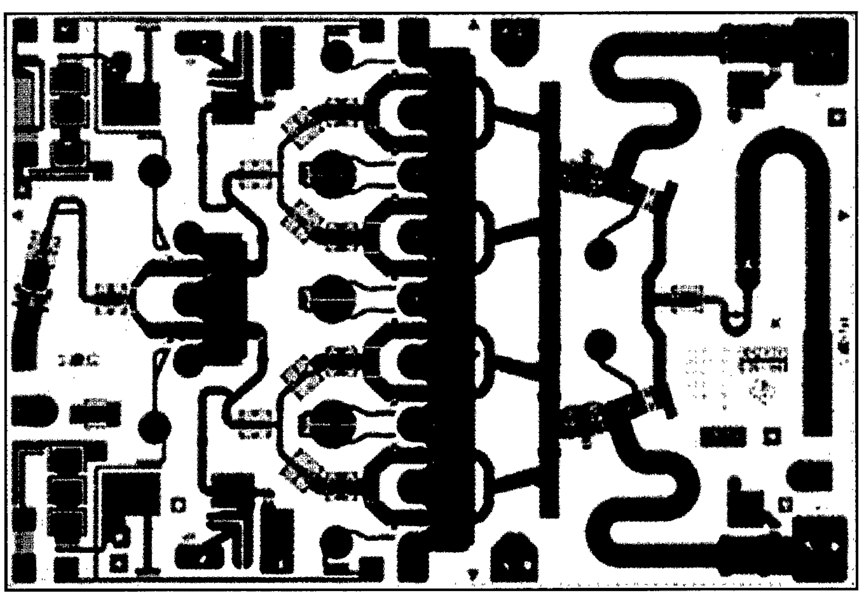
Research Objective: To develop scalable, harmonic-balance simulation for nonlinear, steady-state microwave circuit and system designs that efficiently analyze nonlinear circuit effects within a steady-state regime.

Methodology: Steady-state analysis of nonlinear circuits with either widely varying time constants or significant distributed-element effects is best accomplished with the harmonic balance method. Given a set of analysis frequencies of interest (e.g., a fundamental and several harmonics), the harmonic balance method requires iterative updates to harmonic voltages to reduce the predicted current error between linear and nonlinear circuit elements. Additionally, the code contains several advanced features (including interactive tuning, optimization, and statistical design) that make use of repeated simulations, which also benefit from simulation speed up.

Results: The first effort to parallelize this code was successful, yielding upwards of 98% parallel efficiency on a variety of HPC resources using native message-passing and shared-memory application-programming interfaces. While the approach yielded almost ideal computational efficiency, it was limited in its ability to scale. While the method leveraged the large-grain parallelism inherent to harmonic balance, scalability was limited to the number of frequencies analyzed. The message-passing interface-based effort uses much smaller grain parallelism and thereby achieves much greater scalability. This new method converts the linear hierarchy of subcircuits to be analyzed at each frequency point into a directed acyclic graph (dag) of analysis dependencies. The resultant data-dependency dag, now composed across both subcircuits and frequencies, is then analyzed in parallel, limited only to the true data-dependencies that exist. Furthermore, the method also parallelizes the evaluation of the nonlinear models. The scheduler should operate cognizant of the issues of communication contention, overhead, and latency that exist on each machine. Although good results have been obtained, even better results are anticipated when "machine-dependent" schedulers are developed.

Significance: High-frequency ranges, especially millimeter-wave frequencies, are of utmost importance in a wide variety of DoD remote-sensing, radar, satellite communications, applications, etc. Furthermore, since monolithic microwave integrated circuit (MMIC) fabrication costs are high, "first pass" design success is critical—this mandates not only accurate modeling but requires extensive statistical design as well—placing utmost demand on computational resources.

JWCO: Precision Force, Combat Identification, Joint Theater Missile Defense, Military Operations in Urban Terrain, Joint Countermine, Electronic Combat



Typical MMIC amplifier circuit

Selected References

Parallel Electromagnetic Solvers for High-Frequency Antenna and Circuit Design

J.-G. Yook, B. Perlman, J. Cheng, D. Chen, and L. Katehi, "Parallel Electromagnetic Solvers for High Frequency Antenna/Circuit Design," DoD HPCMP User Group Meeting, San Diego, CA, June 1997.

J.-G. Yook and L. Katehi, "Characterization of MIMICs Packages Using A Parallelized 3D FEM Code," 1996 Advanced Computational Electronics Conference Symposium, March 18-22, 1996, Monterey, CA.

J.-G. Yook and L. Katehi, "Parallelization of the Finite Difference Time Domain Code on Shared Memory Machine," Progress in Electromagnetics Research Symposium 1996, July 15-18, 1996, Innsbruck, Austria.

Nonlinear, Frequency Domain Circuit and System Modeling

D.L. Rhodes and B.S. Perlman, "Parallel Computation for Microwave Circuit Simulation," *IEEE Transactions on Microwave Theory and Techniques*, Vol. 45, 587-592 (1997).

Integrated Modeling and Test Environments

The Integrated Modeling and Test (IMT) Environments computational technology area provides the DoD research, development, test, and evaluation (RDT&E) community with an avenue for advancing the state of test and evaluation (T&E) technology by developing and applying scalable software. HPC software and hardware assets are leveraged to affect current DoD acquisitions by using simulation-based design and acquisition techniques to save time and resources, and to accelerate initial operational capabilities. The same software and simulation tools are used to assess future materiel requirements for the Services. This advanced HPC and simulation capability also provides an efficient capability for data collection, testing, and system analysis within the operational T&E community. Integrated models use multidisciplinary computational techniques with a physics-based tie to the real world to produce infrared and visible spectrum simulations of digital scenes. High-fidelity models are used for one-on-one or few-on-few engagements to evaluate materiel concepts. Simulation-based design allows for rapid insertion of changed concepts to evaluate materiel vulnerability and survivability. DoD materiel undergoes virtual testing throughout its life cycle, from components to subassemblies to full assemblies and systems. The ultimate goal is to reform the acquisition process by providing simulation-based acquisition environments in which hardware prototypes can generally be eliminated.

The IMT success stories here provide examples of major DoD activities using these techniques for process simulation and modeling large composite structures and on-line turbine engine test support.

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CTA Leader for IMT

Integrated Modeling Technology for Process Simulation and Manufacture of Large Composite Structures

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R.V. Mohan and K.K. Tamma
University of Minnesota, Minneapolis, MN

HPC Computer Resource: TMC CM-5 [AHPCRC DC]

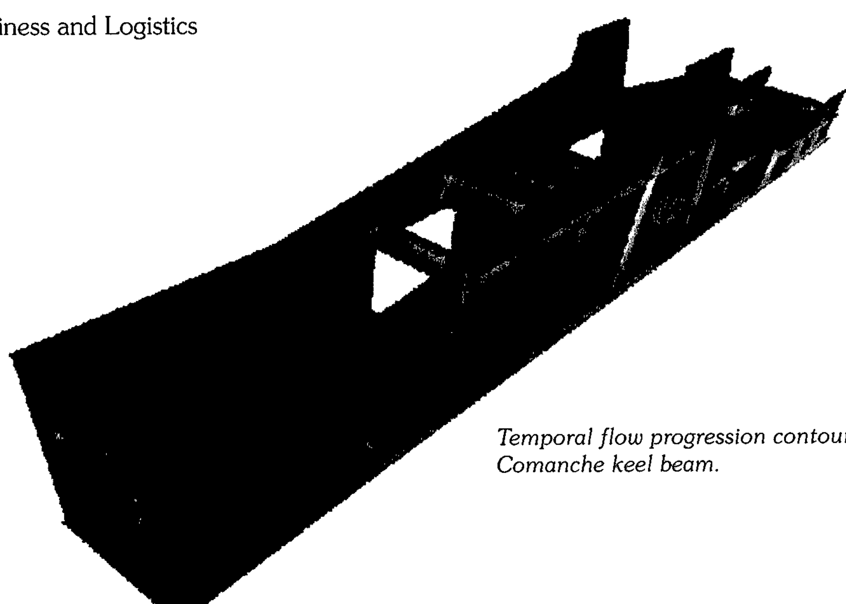
Research Objective: To develop integrated modeling, simulation-based design, and virtual testing methodologies by numerical modeling and simulation of composite manufacturing processes and by analyzing DoD composite weapons platforms for structural integrity and survivability.

Methodology: The prohibitive factors in the development and acquisition of new, composite weapon systems are the cost and limited experience in manufacturing. The integrated modeling environment couples the design, process simulation, and structural integrity analysis to provide a design and production methodology for large composite structures. The processes and analyses are formulated mathematically and the design and acquisition are simulated from these formulations on high performance computing platforms. Thus we contribute materially to a reformed acquisition process as well as to the science and technology base for composite materials and computational technology.

Results: Physical process modeling and simulation of composite manufacturing processes such as resin transfer molding (RTM) pose significant challenges and computational difficulties. New computational methodologies and approaches have evolved for optimal use of the high performance computing resources. Process flow modeling in complex composite structures involving heterogeneous fiber preform is the first step in the process modeling simulations. To this effect, a new, pure finite-element methodology has been developed and has shown significant physical and computational advantages over traditional practices and approaches. Applications of the developments include the 24-foot keel beam section of the RAH-66 Comanche. The figure shows the temporal resin flow pattern and progression.

Significance: This technology contributes significantly to joint readiness by providing the warfighter with an affordable, lethal, and survivable product. RTM is a net-shape composite manufacturing technology with a significant potential for cost-effective manufacturing of large composite structural parts. The understanding of the resin progression in complex shapes, such as the 24-foot keel beam section of the RAH-66 Comanche, permits the determination of optimal process parameters avoiding dry spot formation and piece-part rejections during manufacture, which leads to process maturation and shorter product development times. This is the first time that RTM process simulations in such structures have been computationally modeled. Manufacture of large complex parts such as the composite keel beam benefit significantly from the integrated modeling technology approaches leading to faster acquisition cycle times. Furthermore, this technology has a ready dual-use utility for the transportation industry by strengthening their industrial base with relatively little expenditure of internal funds.

JWCO: Joint Readiness and Logistics



Temporal flow progression contours in 24-ft Comanche keel beam.

On-Line Turbine Engine Test Support

J.B. Thompson and R.L. Zarecor
Arnold Engineering Development Center and Sverdrup Technology Inc., Arnold AFB, TN

HPC Computer Resource: Convex C4640, C3880, and SPP-2000 [AEDC DC]

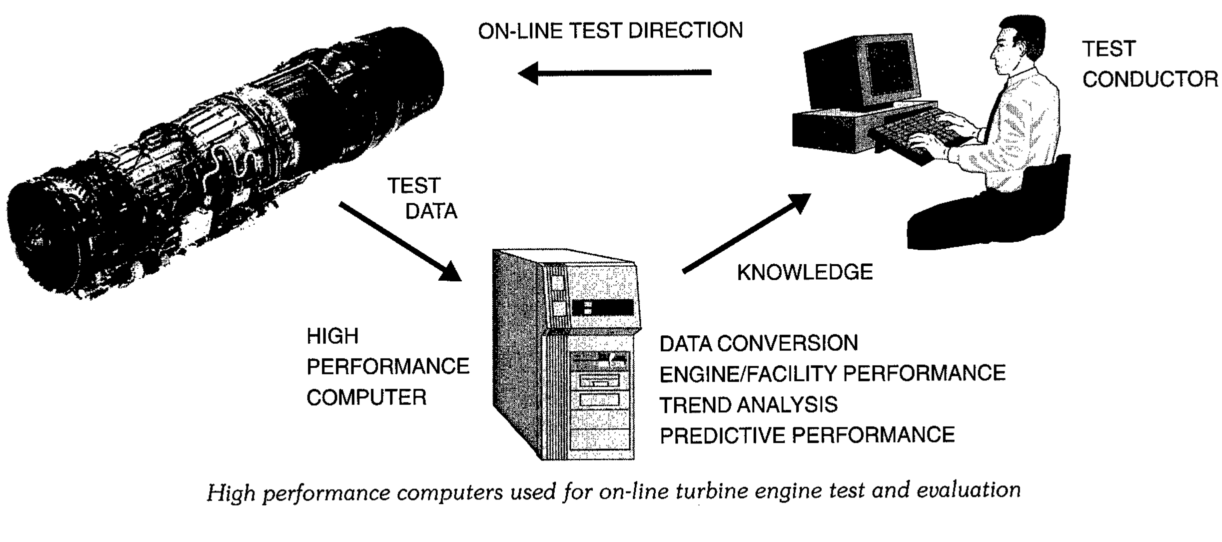
Research Objective: To provide processed turbine engine test data in near-real time to enable timely test direction decisions. Facility operation hours for turbine engine testing are very expensive ($10,000/hr for the smaller test units up to $27,000/hr for the larger test units). Processing test data on-line allows the test conductor to make critical decisions during the test, preventing expensive future retesting. In addition, processed test data are available for detailed analysis and reporting much sooner than when using conventional solutions. This concept was developed in 1986 with the delivery of the Aeropropulsion Systems Test Facility (ASTF) and expanded over the years to include all of the Engine Test Facility (ETF) turbine engine test units.

Methodology: The on-line near-real-time processing concept was initiated with the delivery of the ASTF test units in 1986. This concept incorporated array processors in the data acquisition stream to convert raw test data to engineering units (EU) data. The EU data were then sent to a Cray-1s system for calculation of engine performance parameters. Performance data were then sent to Apollo workstations for on-line analysis and to the central archive facility for future access. These computer systems were networked together with a high-speed (50 millibits per second) hyperchannel network. Upgrades from the original concept have included three processing system upgrades (Cray X-MP in 1991, a Convex C3840 in 1993, and a Convex C4640 in 1996), a network upgrade from proprietary hyperchannel to industry standard Ethernet and FDDI, and an analysis system upgrade from Apollo workstations to Sun and SGI UNIX workstations. A preemptive priority scheme was installed in 1989 allowing unused computer cycles to be shared with nontest support customers.

Results: Test data point turnaround time decreased from an average of 10 minutes to 2 minutes. This concept was targeted for the F119 engine development tests in ASTF but has been expanded to all the turbine engine test units in the ETF. Some of the programs supported were F119, F100, F110, F414, F402, F404, Pratt & Whitney 4000, and Rolls Royce Trent engines. While difficult to quantify, using on-line data processing is estimated to have provided a cost avoidance of $46 million since its inception in 1986. In addition, customers are pleased with the improved response provided by this approach because validated test results are available much sooner than with previous approaches. Also, maintenance and reliability have improved through the use of industry standard hardware and systems. The preemptive priority scheme has provided computer resources to nontest customers that would not have been available otherwise.

Significance: This data processing concept has provided processed data for on-line test direction for several major propulsion system test programs. A significant cost avoidance has been achieved while providing the test customer faster access to engine performance results. With new technology computer systems and networks, continued improvements in this area are expected.

JWCO: Precision Force, Joint Readiness and Logistics



High performance computers used for on-line turbine engine test and evaluation

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